NASA Research Grant NsG-398

Computer Oriented Research in the Space Related Sciences

Annual Status Report

March 1965 to February 1966

Werner C. Rheinboldt

Dr. Werner C. Rheinboldt
Principal Investigator
Computer Science Center and
Institute for Fluid Dynamics
and Applied Mathematics
University of Maryland

Azriel Rosenfeld

Dr. Azriel Rosenfeld
Co-principal Investigator
Computer Science Center
University of Maryland

Table of Contents

B. Computer-oriented research projects in other space-related fields
   1. Molecular physics and astronomy
   2. Nuclear physics and engineering
   3. Physics and engineering of fluids
   4. Physics and astronomy
   5. Other computer-oriented research in the sciences
   6. Other computer-oriented research in engineering

Appendix

I. Computer time summary

II. Computer time supported by NASA Grant NsG-398

III. Publications, reports and theses resulting from research which received computational support under NsG-398

Chapter I

INTRODUCTION

A. Objectives

In March, 1963, the National Aeronautics and Space Administration awarded research grant NsG-398 to the Computer Science Center of the University of Maryland. This grant, entitled "Computer Oriented Research in the Space-Related Sciences", was given in support of a broad multi-disciplinary research program which is aimed at stimulating and broadening the effective use of large-scale computers in the University's extensive space research efforts, and at investigating new methods of computer applications in these fields.

In line with the above stated aims, the research program being conducted under the Grant involves two interrelated areas of activity:

1) Research in the computer sciences with the goal of deepening knowledge and understanding of the most effective use of computers in research. This includes work on the design and implementation of programming and monitoring systems and their properties, research on special algorithmic languages and their compilers, as well as research in such areas of the computer and information sciences as image processing and automatic pattern recognition, information storage and retrieval systems, and computer-oriented mathematics.

2) Support of the computer-oriented phases of a broad spectrum of space-related research projects in close cooperation with investigators in many different academic disciplines. Such interdisciplinary research ranges from the analysis of methods for an effective computational approach to a problem, to the development of special techniques and programs.

It should be emphasized that Grant funds are used only in support of the computer science aspects of the projects referred to under (2). While many of these projects have partial support from other sources, in no case do they have support for related computational work or associated computer science research. In several cases, projects which initially received support under the Grant have obtained independent support for their computational phases, and so are no longer receiving Grant support. Such success by collaborating investigators is welcomed, particularly in those instances where the success of the initial

computational work supported by the Grant was instrumental in helping to obtain the independent support.

When a computer is used as part of a research project, the high cost of the necessary equipment, problems of securing proper programming help, etc., often overshadow the entire computational effort and overstress the service nature of the computer work. At the same time, any serious research investigator knows that this service aspect is not the major consideration associated with the really effective application of computers. A very significant contribution stems from the fact that the analysis undertaken to make possible the assistance of computers will often stimulate a type of feedback that casts new light on the research problem itself, thereby in turn serving to further the research effort. It is an aim of the Grant program to stimulate this type of thorough analysis in the computer science aspects of the individual projects being supported under the Grant and thereby to bring to the investigator's awareness the potential new approaches to his problems made possible by the use of modern computers.

The research results obtained so far under the Grant have been reported in the form of 25 research reports of the Computer Science Center and more than 70 publications and presentations. In addition, a growing number of graduate students from various departments are actively participating in research work under the Grant and pursuing research studies which involve use of the computer as part of the requirements for an advanced degree. As of November 1965, 23 students had already completed studies of this type, 9 of them receiving a Ph. D. degree, and 14, a Masters degree. Over 40 other such projects are currently under way.

In general, it can be said that during the past four years, space-related research activities at the University have expanded rapidly and have achieved increasingly widespread recognition. This research necessarily involves extensive use of large scale computers. More important, effective application of modern computational theory and methods in such research depends greatly on advances in the computer sciences themselves and on close cooperation between computer scientists and research workers in the space sciences. The Grant provides a unique opportunity for such multi-disciplinary activity of the type most conducive to effective space oriented research, and it has stimulated a close collaboration between computer scientists and investigators in a wide range of disciplines. Initially, the Grant also provides partial computational support to investigators who have not been able to obtain it

otherwise. As the investigator gains familiarity with high speed computing capabilities, he is encouraged to formulate his computational problems in the broadest possible terms. The results can then be embodied in a flexible programming system which in turn can be used by other investigators in the same field. Parallel with this, the active research work in basic problems of the computer sciences themselves now under way at the Center would not have been possible without the support of the Grant. In fact, the support of the Grant has been one of the most significant factors in the development of the entire Computer Science Center into a successful research organization in the short span of four years.

B. Scope of this report

A continuation of Grant NsG 398 was awarded to the Computer Science Center effective March, 1964 and a further continuation effective March, 1965. Throughout this period, intensive work has continued in both areas of the research program. Reports on the projects which have been supported under the program during the reporting period just completed, through January 1966, are presented in Chapter II. An overview and summary of these projects is presented at the beginning of that chapter. In addition, lists of the individual projects within each research area are given at the beginnings of sections within Chapter II.

Many of the projects which have been given computer support under the Grant are master's thesis and doctoral dissertation projects in the Graduate School of the University. Reports on these thesis projects are included together with the reports on faculty research projects in Chapter II. Lists of the completed thesis projects and of the thesis projects in progress are given as part C of Appendix III. Parts A and B of that appendix list Computer Science Center Technical Reports and other selected reports, presentations and publications which have resulted from research supported by the Grant.

For each project in Chapter II, figures are given showing the computer time used at the Computer Science Center during this reporting period, as well as the total computer time used by the project since its inception.* These figures are summarized in Appendix II by major group of projects or department,

---

*These figures do not include computer time supported by other outside sources, which amounted (for these projects) to about 1% of the time reported here.

as appropriate, for each month in the period February 1965 through January 1966. For comparison purposes, the total computer usage at the Center by college and month over the same period is given as Appendix I. (Figures for February 1966 were not available in time for inclusion in this report.) During the reporting period, an average of only about 49% of this computer time was billed to NASA under the Grant, as detailed in Appendix II; the remainder was supported by the University.

C. Personnel

This section lists the Computer Science Center personnel who have made major direct contributions to the research being conducted under the Grant.

Dr. Werner C. Rheinboldt, Research Professor of Computer Science, continues as the principal investigator for the entire program. Effective July, 1965, Dr. Rheinboldt resigned his position as Director of the Computer Science Center in order to devote full time to research activities.

Dr. Rheinboldt is also directing the research projects in numerical analysis, with the assistance of Dr. James M. Ortega, Research Assistant Professor of Computer Science; Dr. Abraham A. Tal, Visiting Research Assistant Professor of Computer Science; and Mr. James S. Vandergraft, Research Associate. Dr. Richard H. Austing, Assistant Professor of Computer Science, is responsible for program evaluation work in numerical analysis. The programming support for this research is headed by Mr. Charles K. Mesztenyi, Senior Research Programmer, whose programming group includes Messrs. Robert L. Clark and Zalman A. Shavell, Research Programmers.

Dr. Azriel Rosenfeld, Research Associate Professor of Computer Science and co-principal investigator for the program, directs the image processing and pattern recognition research, with the collaboration of Dr. Nancy S. Anderson, Associate Professor of Psychology and Research Consultant at the Computer Science Center. Dr. Robert C. Glasser, Associate Professor of Physics and Computer Science, heads the nuclear bubble chamber pattern recognition project. Programming support for this research is provided by Mr. John L. Pfaltz, Senior Research Programmer, together with Mr. John M. Johnston, Junior Research Programmer. Mr. Pfaltz is also responsible for the research on tree and graph-structured data.

Dr. Earl J. Schweppe, Associate Professor of Computer Science, is directing research on ALGOL and on non-sequential procedures. Mr. Howard D. Wactlar, Research Programmer, has provided programming support for this work, and is also developing the graphic man-machine system for on-line data analysis.

The programming systems development work is under the direction of Mr. Alfred E. Beam, Senior Computer Systems Analyst, with the close cooperation of Mr. John P. Menard, Acting Director of the Computer Science Center, and the assistance of Mr. Robert J. Herbold, Computer Systems Analyst. Valuable support to this work has been provided by Mr. Gerald M. Berns, IBM Corporation Systems Engineer.

Mr. Chan M. Park, Research Programmer, is developing the Chemical Engineering Programming System. Mr. James F. Williams, Research Programmer, is responsible for the work in statistical programming.

The staff of the Computer Science Center is not only responsible for conducting the computing systems and computer science research work described above, but also contributes to the computational phases of the other projects in these and other space-related fields which are receiving computer support under the Grant. The principal investigators of the individual projects, and their departmental affiliations, are given together with brief project descriptions in Chapter II.

The following Graduate Research Assistants were associated with the program during the fall semester: Stephen Herman, Robert Lieberman, Robert Voight, and Louise Zembiski. Three of the University's 30 NASA trainees, John L. Maryak, Richard Elkin, and Joseph Caspar, are working in computer oriented mathematics.

D. Facilities

The entire research program being supported by the Grant involves extensive large-scale computer use. This computer support is provided through the facilities of the Computer Science Center. At the start of the program, the Center was provided by the University with an IBM 7090/1401 system and associated card handling equipment. In September 1964 the 7090 was converted to a 7094. A second 1401 was installed in November 1964. This added equipment, the acquisition of which was supported in part by a National Science Foundation Grant, has considerably improved the overall speed, computing power

and efficiency of the installation.

An extension to the Computer Science Center building, which provides approximately 9000 square feet of additional space, was opened for occupancy in May 1965.

Chapter II

DETAILS OF THE RESEARCH WORK

This chapter describes the individual research projects which were conducted under the Grant program.

As indicated in Chapter I, the research which has been performed under the program is of two types:

A. Research on problems in the computer and information sciences, and development of programming systems for computer utilization in space-oriented fields

B. Research on the computer-oriented phases of a broad spectrum of space-related research projects, in close cooperation with investigators in many different disciplines

The first part of this chapter describes research areas of the first type. The following is a brief summary of these areas:

Area	Brief description
(1) Computing and programming systems development	
(A) Programming systems	Continuing effort to develop general purpose programming systems, with emphasis on flexibility of access to the computer by researchers
(B) Crystallographic computing system	Development of a major computing system for crystallographic structure analysis, which has found widespread acceptance throughout the world
(C) Electrolyte data computing system	Development of a versatile, self-contained computing system for research on electrolytes
(D) Computing system for solution kinetics	Integration of a variety of programs for analyzing chemical reactions in solution

(E) Programming systems for numerical analysis	New project devoted to evaluation of languages and routines designed for use in numerical analysis
(F) Computing system for chemical engineering	Development of a unified package of general and special purpose subroutines useful for the solution of problems in chemical engineering
(G) Statistical computing systems	Development and evaluation of programs for statistical analysis of data
(H) Management information structures	Study of PERT systems (being suspended)

(2) Computer and information sciences research

(A) Numerical analysis	Numerical solution of non-linear operator equations; integral equations; eigen-value computations; numerical approximation and integration
(B) Image processing	General purpose digital image processing techniques; image syntax; applications to cloud cover pictures, nuclear bubble chamber pictures, maps
(C) Visual perception and pattern recognition	Studies of the perception of visual texture, form and pattern, using the computer both to generate complex stimuli and to formulate models for perceptual pro-cesses
(D) Procedure languages and system structures	ALGOL implementations; con-sequent procedures; tree structure processing

(E) Visual display man-machine interaction	New project to develop graphic man-machine system for on-line analysis of experimental data
(F) List processors and tree-structured data	New project aimed at developing a system of subroutines for manipulating data trees; planned extension to graph-structured data
(G) Experimental algebraic number theory	Computational approach to algebraic number theory with goal of obtaining new insights and formulating new conjectures
(H) Information storage and retrieval	Study of information structures useful for retrieval in depth in a specialized subject area

Over eighty research projects of the second type were active or approved for support during the reporting period just completed. Brief summaries of the new projects of this type are presented in the second part of this chapter. For continuing projects, and for those completed during this period, summaries may be found in previous Status Reports; the present report updates these summaries as required. These projects are grouped under six headings as follows:

Field	Departments or sections represented	Number of projects
Molecular physics	Chemistry, molecular physics, fluid dynamics	16
Nuclear physics and engineering	Nuclear physics, chemical engineering	25
Physics and engineering of fluids	Aerospace engineering, chemical engineering, fluid dynamics, atmospheric and space physics	17
Physics and astronomy	Astronomy, solid state physics, particle physics, atmospheric and space physics	14

Other sciences	Biophysics, experimental psychology, medicine	7
Engineering	Aerospace, civil, electrical and mechanical engineering	11

Under each heading, individual projects are presented in three groups: new projects; continuing projects; and projects completed during or shortly before the current reporting period. Within each group, the projects are given in reverse order of date of initiation, beginning with the most recent. Computer time is given in hours and minutes, rounded to the nearest minute. The information is complete through January 31, 1965.

A. Computing systems and computer science research

1. Computing and programming systems development

(A) Programming systems

Principal investigators

Mr. Alfred E. Beam	Senior Computer Systems Analyst	Computer Science Center
Mr. John P. Menard	Acting Director	Computer Science Center

In cooperation with

Mr. Gerald M. Berns	Systems Engineer	IBM Corporation

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/65/002	Systems engineering IBJOB-IBSYS	1/65	12/65	12/12	12/28
001/65/003	Systems work	1/65	Continuing	126/1	151/27
001/66/002	Systems engineering IBJOB-IBSYS	1/66	Continuing	0/8	0/8

Publication (during reporting period):

Computer Science Center Technical Report TR-65-25, FORTRAN II to FORTRAN IV Translator UOM SFT for the IBM 7090/7094, by Donald E. Eastlake III, November 1965

(1) IBSYS

The overall operation of the three primary systems (IBJOB, MAMOS, and FORTRAN II) under IBSYS was considerably improved by re-arrangement of components on the two library system tapes. With this arrangement and the fast FORTRAN IV compiler, IBJOB is a very efficient monitor system.

(2) IBJOB

MIMIC, a system for solution of ordinary differential equations, was put on the IBJOB library so that it is easily

called and may be used in courses. The double precision routines of IBLIB which use 7094 instructions were assembled and now replace the 7090 versions. The routines were extensively checked by a job which created a tape of x, f(x) in selected ranges for each of the functions. The tape was written with PRECISE statements intermixed in the output so that it was a suitable input tape for the PRECISE system. A PRECISE job was then run with the previously generated tape as input. Each f(x) was computed by PRECISE, and x, the two values of f(x), and the differences between the two values were printed. Also, a fast internal sort subroutine was prepared and entered into IBLIB.

An editor deck and procedure were given to several users who have extremely large programs (or many small programs) so that they may create their own IBLIB. In running their programs, they ask for their library to be mounted, and via IBSYS Control Cards, they cause their library tape to replace the regular library tape for IBJOB. The maximum number of control sections on any one library is still too limited to be entirely satisfactory, and it is hoped that this restriction can be removed in the future.

(3) OMNITAB

All input-output of OMNITAB has now been replaced and other changes have been made so that a single version will run under either stand-alone or direct-coupled versions of IBSYS. This version is the one now under UOM IBSYS, and the same version has recently been installed on the direct-coupled system of Goddard Space Flight Center. The mathematical subroutines of OMNITAB were also considerably improved.

(4) PRECISE

Several operations were added to PRECISE, and it was modified to work on either stand-alone or direct-coupled systems. PRECISE was recently installed on the direct-coupled system of Goddard Space Flight Center. A write-up for the system is in progress.

(5) MAMOS

The system was requested by and sent to several installations. The latest version, which included the new MAD translator and SNOBOL, replaced the older version in operation at Goddard Space Flight Center. The SNOBOL language program

(UOM SFT) for translating FORTRAN II to FORTRAN IV source programs was completed and the report mentioned above was published. The program, though slow, is proving quite useful because of the additional features not available in other programs of this type.

(6) IBM 360 Work

Most of the initial version of a 360 utility program was written and should be operational when the IBM 360-Model 30 is installed in March, 1966. The program is written to provide input-output support for the IBM 7094. It is capable of printing or punching from two tapes and at the same time doing a card to tape operation. Other operations will be added in the future.

The monitor for the Basic Operating System for 360 was studied and a small version of the program was written to operate on the 7094 via the SUPPAK system under IBSYS. This allows most of the check-out of the utility package to be done without having access to a 360.

(B) Crystallographic computing system

Principal investigators

Dr. James M. Stewart	Associate Professor	Chemistry
	Research Consultant	Computer Science Center
Dr. Albert Hybl	Assistant Professor	Biophysics

Project No.	Title	Initiated	Completed	Computer time Reporting period	Total
201/64/003	X-ray diffraction	10/64	In progress	149/31	232/44
455/64/002	Crystallographic programs	11/64	In progress	20/48	22/58

During the period 15 November - 12 December, the principal investigator supervised the installation of an operational X-RAY system on the IBM 7090 at Imperial College, University of London. This trip was sponsored by Mrs. Olga Kennard of the Cambridge University Chemical Laboratory.

The system has also been installed at the IBM Data Centre and Unilever Research Laboratory in London. Symbolic programs have been delivered to Hartwell for translation to HARTRAN for the Atlas computer.

(C) Electrolyte data computing system

Principal investigator

Dr. Gordon Atkinson — Associate Professor — Chemistry

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
201/63/002	Conductance of charge-separated electrolytes	1/64	In progress	0/35	2/43
201/63/003	Ion association in polyvalent electrolytes	11/63	In progress	0/36	6/3

Publications (during reporting period):

G. Atkinson and S. Petrucci, J. Phys. Chem., in press (1966)

G. Atkinson and S. K. Kor, J. Phys. Chem., in press (1966)

G. Atkinson and S. K. Kor (to be presented, Pittsburgh ACS meeting, March 1966)

G. Atkinson, S. K. Kor, S. Petrucci, Proc. IEEE, 53, 1355-1362 (1965)

This research project involves an extensive program of measurements and theoretical calculations of electrolyte solution properties. Measurements are being made of conductance, transference numbers, Wien effect dispersion, and ultrasonic absorption and dispersion. The theoretical calculations are concerned with conductance and its related irreversible thermodynamic properties, and with the kinetic, thermodynamic and structural interpretation of ultrasonic transmission parameters in solution. In the case of conductance particular attention is being paid to the critical comparison of the various theories proposed to explain electrolyte conductance.

The most important computational problems being attacked at present will be described in the following paragraphs.

(1) Ultrasonic absorption

Each equilibrium or equilibrium step present in a

chemical system can be described by a single relaxation equation of the form

$$\mu_i = 2\mu_i^* \left(\frac{\omega \tau_i}{1 + \omega^2 \tau_i^2} \right)$$

where μ_i = absorption of sound per wavelength

μ_i^* = maximum absorption per wavelength

τ_i = relaxation time

ω = angular frequency = $2\pi f$

For a system containing a number of processes the μ at any ω is given by

$$\mu = \Sigma_i \ \mu_i$$

The basic problem is to treat the (μ,ω) data set so as to yield a μ_i^* and a τ_i for each process. For a system where there are N processes, (N-1) can usually be detected by simple visual inspection.

Data processing steps

Step A
1. Treat raw data (db_j, X_j) to yield α (absorption coefficient) at given f.
2. Calculate α/f^2, λ, $\alpha - \alpha_s = \alpha'$ and $\mu \equiv \alpha'\lambda$.

Step B
1. Fit (log μ, log f) data to polynomial series.
2. Obtain preliminary (μ^*, τ) by polynomial differentiation.
3. Refine (μ^*, τ).

Step C
1. Modification of Steps A,B for multiple relaxations using expansion around estimated values.
2. Calcomp plotter analysis.

Step D Calculation of kinetic parameters from τ_i data.

Step E Calculation of thermodynamic parameters from μ^* data.

At the present time Steps A,B and D (partially) have been

programmed, debugged and checked out on real data. Progress is being made on Steps C,E and Step D refinement for more complex kinetic systems.

(2) Conductance and related phenomena

The following theories are being used as the basis for the analysis of high precision conductance and transference number data

a. Fuoss-Onsager (1959)
b. Pitts (1955)
c. Falkenhagen-Leist-Kelbg (1958)
d. Kubo-Friedman (1964)

The first has been completely programmed in a very general form so that numerous theoretical adjustments can be made. Programs involving the Pitts theory have developed some problems which are not yet resolved. Work is progressing on the programming of the FLK theory, which seems to be very straightforward. The Kubo-Friedman theory presents much greater computational problems than the other three. It will involve the evaluation of large numbers of "cluster" integrals by iteration techniques. At the present time an attempt is being made simply to program it as a theoretical calculation without attempting to use it for data processing. This latter phase must await the development of some rather subtle subroutines.

At the present time subroutines have been developed so that all conductance calculations can be made from raw data input: weights, measured resistances, solvent parameters.

(3) Pressure-jump calculations

The recent development of a pressure-jump apparatus in this laboratory has necessitated the development of a program in P-jump data calculation and related relaxation kinetics. In the pressure jump a chemical equilibrium is perturbed by a 50 atm pressure. The pressure is suddenly released and the return of the system to its 1 atm equilibrium position monitored by conductance. The computational problems are:

(a) Analysis of relaxation conductance data to yield τ values (relaxation times).

(b) Interpretation of τ values in terms of the kinetic parameters of multi-step relaxation processes.

Work is progressing on Step (a) programming. The calculations of Step (b) are very similar to these used in ultrasonic analysis. In this case ultrasonic calculation subroutines are being modified to accept P-jump data input.

(D) Computing system for solution kinetics

Principal investigator

Dr. Gilbert Gordon — Associate Professor, Chemistry
Research Consultant, Computer Science Center

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
201/65/005	The kinetics of the oxidation of chromium (II) by chlorate in aqueous perchloric acid	1/65	3/65	0	0/10
201/65/006	Mechanisms and equlibria in inorganic reactions	2/65	In progress	85/59	86/12

Publications (during reporting period):

G. P. Haight, Jr., E. Perchonock, F. P. Emmenegger, and G. Gordon, The Mechanism of the Oxidation of Sulfur (IV) by Chromium (VI) in Acid Solution, J. Am. Chem. Soc. 87, 3835 (1965)

B. Z. Shakhashiri and G. Gordon, Oxygen-18 Exchange Reactions Between Gaseous Oxygen and Certain Oxygen-Containing Inorganic Salts, J. Inorg. Nucl. Chem. 27, 2161 (1965)

G. Gordon and P. H. Tewari, The Kinetics of the Reaction Between Vanadium (II) and Chlorate in Aqueous Perchloric Acid, J. Phys. Chem. 70, 200 (1966)

During this reporting period, considerable effort has been devoted to the development of methods for routinely solving data handling problems associated with the reactions and interactions of dissolved species in aqueous solution. This report summarizes progress in four specific areas.

(1) Non-linear data fitting system

The program discussed in this section is described in detail in Los Alamos Scientific Laboratories Publication

LASL-2367. Appreciation is expressed to R. Moore and T. W. Newton of LASL for making it available.

The capacity of the program is as follows:

Number of independent variables (m)	5
Number of data points $(y_i, x_{5,i})$	500
Number of parameters (p_i)	30

The general purpose of the program is to make least square fits of data to arbitrary functions by the Gauss method. In this method, the function is linearized with respect to each of the parameters by means of a truncated Taylor series. Using initial estimates of the parameters, the coefficients of the expansion are evaluated and new estimates obtained. The process is repeated until a convergence criterion is satisfied.

The following are functions which can be linearized by subroutines of the program:

$IBFTC deck	Function to be linearized
Y002	Sum of exponentials
Y053	Multiterm activation energy for parallel rate law
Y114	Gaussian fit for sum of up to five curves
YTRIP	Sum of polynomials
YNEW1	Generalized solution for combined first and second order rate law
GG01	Modified Debye-Huckel equation
GG02	General solution for linear data fitting with polynomial equation
GG03	Five term solution for Young's modulus equation
GG04	Basic solution for diffusion reaction
GG05	Five term solution of GP with use of Young's modulus data
GG06	Generalized solution for polynomial fit of dependence of rate constant on hydrogen ion concentration
GG08	Revised version of GG04
GG09	Equation relating specific rate constant to pressure for gas phase reactions
GG10	One term exponential equation

The following subroutines are currently used in the curve programs:

Name	Function of subroutine
AXIS	Scales axis size, prints axis information
CALC1	Performs calculations for linearization of appropriate YPS subroutines
CHANGE	Recognizes requests for multiple iterations
CKDUMP	Determines status of programs, calls for necessary pdumps
CKPLOT	Initiates HPLOT, SCPLOT and Calcomp routines
CKSSWT	Checks position of sense switches, gives appropriate warning messages
CURVE	Calls for input, output, function, calculation and plot routines
DEFINE	Contains complete descriptions of programs, calling routines, and setup procedures
FIT	Updated version of CURVE
GGPLOT	Constructs arrays for SCPLOT and HPLOT
HASH	Trap routine
HASH2	Prints error message...does not compute... try again
HPLOT	Used to prepare off-line 1401 plots from arrays constructed in CALC1
INPUT	Handles input data; used by FIT and NLLS66
INPUT5	Handles input data; used by CURVE and NLLS65
INPUT9	Handles input data from utility tape units only
LINE	Plots data arrays constructed in SCALE
MATRIX	Does necessary matrix calculations and inversions for error estimation
NLLS65	Main calling program for CURVE
NLLS66	Main calling program for FIT
NUMBER	Used to output numeric data on Calcomp plots
OUTPUT6	Produces most of the normal output
PLT673	Calcomp plot routines
SCALE	Determines necessary scale factors
SCPLOT	Scaling routine for HPLOT
SEARCH	Called to skip to new data set
SYMBOL	Used to output alphanumeric data for each Calcomp plot
TAPES	Checks necessary tape assignments for validity under monitor
UNIT16	Assigns appropriate system tape designations
XGPLOT	Calls all Calcomp routines
YPS	Gives the function to be fitted and its derivatives with respect to each of the parameters
ZAP	Compares two sets of data

(2) Kinetics of the formation of complex ions

The rate of formation of complex ions of the first transition series has been studied by a variety of methods. It is believed that the rate of formation is never faster than the rate of elimination of water from the first coordination sphere of the hydrated transition metal ion. This suggests a mechanism in which a ligand replaces a coordination site cleared by the dissociation of one water molecule.

The rate of water exchange for the first coordination sphere of the ions Mn^{++}, Fe^{++}, Co^{++}, Ni^{++} and Cu^{++} has therefore been of interest. Previous results have been obtained by Connick and Swift by means of wideline nuclear magnetic resonance studies of the oxygen isotope 17 in water and solutions of the paramagnetic ions.

In general, the interpretation of these results is unambiguous. However, in the case of Cr(II) and CU(II) the presence of the Jahn-Teller configurational distortion renders interpretation difficult, since it appears that two out of the six water ligands (the axial ones) are bonded less tightly than the remaining four equatorial ones. It is therefore of interest to measure the rate of exchange of water in an ion such as CuL^{++} or CuL_2^{++} (L=bidentate ligand) where water exchange is only possible at four or two coordination sites respectively. In practice the rate of exchange can be measured as a function of the number of free coordination sites. Obviously the results will also contribute to the elucidation of the mechanisms of formation steps of the ionic species CuL_n^{++}, and possibly even to the stereochemical course of these reactions. In any case it should be possible to observe the rate of the water exchange at specific coordination sites rather than the joint contribution of both the equatorial and axial positions.

For the experiments described, the concentrations of the exchanging species must be carefully controlled. The ligands 1-10 - phenanthroline and 2,2' - dipyridyl appear to satisfy the necessary requirements. The distribution of the species CuL_n^{++} (n = 0,1,2,3) at any given concentration of free ligand, total concentration of metal ion and hydrogen ion ($C_{Cu^{++}} \times C_H$)

is given by the formation constants K_n in the equilibrium

$$M^{++} + L \overset{K_1}{=} ML^{++} + L \overset{K_2}{=} ML_2 + L \overset{K_3}{=} MLs$$

and the formation constant K_B of the protonated ligand. If the enthalpy and entropy of formation for each step are known, the equilibrium concentration of each species and the pH of the solution may be calculated numerically as a function of temperature. A program for the IBM 7090/94 computer was developed and successfully tested.

The addition of paramagnetic salts broadens the n.m.r. lines of oxygen-17 in water since the transverse relaxation time is shortened. Other factors may also influence the line width of an n.m.r. signal. These are insufficient homogeneity of the magnetic field, instability of the magnetic field, saturation of the nuclear system and contributions from transfer of resonating nuclei between magnetically different environments in bulk water.

In H_2O the oxygen-17 resonance is split into a triplet. Exchange of H^+ results in one line which will be broadened if the exchange process becomes too slow. These contributions have to be ruled out by careful selection of experimental conditions. If there is no "artificial" broadening and exchange other than the one between bulk water and ion contributing to the linewidth, meaningful data can be obtained. The contribution of the paramagnetic ion to the width of the resonance line itself may then be controlled by the rate of chemical exchange, by the slowness of the nuclear relaxation in the first coordination sphere of the ion, or the slowness of relaxation in the bulk water. Whenever the overall relaxation process is controlled by chemical exchange, the logarithm of the broadening effect of the paramagnetic ions of the water resonance line is proportional to the reciprocal of the absolute temperature (Arrhenius type of behavior). Thus it can be determined whether the overall relaxation is controlled by the exchange process or by the relaxation process.

(3) Combined first and second order rate law

Preliminary calculations for the chromium(II)-chlorate system indicated that at constant hydrogen ion concentration the kinetic data were consistent with a second order rate equation, first order each with respect to chromium(II) and to chlorate ion. The data were analyzed by means of two independent computer programs.

(A) Linear least squares program:

The chromium(III) products of the halate, chromium(II) reactions $(H_2O)_5CrCl^{++}$, $Cr(OH_2)_6^{+++}$, and the polynuclear species, all exhibit very similar absorption spectra in the visible wavelength region but do not show an isobestic point. Therefore, an effective extinction coefficient, E_{eff}, was defined:

$$E_{eff} = (A_\infty - A_0)/(1 \times N)$$

where A_∞ = infinite optical density
A_0 = initial optical density
1 = path length (cm.)
N = normality of reactant not in excess

The chromium(III) concentration at any time t, Cr_t^{+++}, was then calculated from the Beer's Law relationship:

$$Cr_t^{+++} = (A_t - A_0)/(1 \times E_{eff})$$

where A_t is the optical density at any time t. The chromium(II) and the chlorate ion concentrations were calculated for thirty different values of the recorded transmittances for each run.

The initial transmittance observed was corrected for a dilution of the small amount of absorbing chromium(III) in the cell upon injection of the transparent sodium chlorate solution. The A_o corrected value was calculated from the relationship:

$$A_o \text{ corrected} = 0.915_5[A_o - A_{cell}] + A_{cell}$$

where 0.915_5 is the ratio of volumes prior to and after injection and A_{cell} is the cell correction for the reaction cell filled with distilled water. These corrections were very small, since the initial transmittance was usually > 90%, and the injected sodium chlorate diluted the solution by only about 10%. In a typical run, 0.064 and 0.060 absorbance units were the uncorrected and corrected respective initial absorbances.

When the chromium(II) - chlorate reaction was followed by observing the disappearance of chromium(II) at 7190 Å, the same method of calculating concentrations was used. In this case,

however, a somewhat larger dilution correction for the initial absorbance resulted, owing to the larger initial value.

The linear least squares program calculated the rate constant k_1 appropriate to the integrated second order rate expression:

$$\ln[Cr(II)_t/(ClO_3^-)_t] = [(Cr(II)_o/6) - (ClO_3^-)_o]\, k_1 t + \ln[Cr(II)_o/(ClO_3^-)_o]$$

where k_1 is the second order rate constant (M^{-1} sec^{-1}).

$[Cr(II)]_t$ is the chromium(II) concentration at time t,

$[Cr(II)]_o$ is the chromium(II) concentration at t = 0,

$[ClO_3^-]_t$ is the chlorate ion concentration at time t,

$[ClO_3^-]_o$ is the chlorate ion concentration at t = 0, and

t is the time in seconds.

The best linear fit was determined analytically for the $\ln\{[Cr(II)]_t/[ClO_3^-]_t\}$ as a function of time by standard least squares techniques.

(B) Nonlinear least squares program:

This program differed in several important respects from the linear least squares program. The best nonlinear least squares fit* of the data with the second order rate equation was found by minimizing the quantity $(A_{obs.} - A_{calc.})^2$ where $A_{obs.}$ is the observed optical density and $A_{calc.}$ is the calculated optical density from the parameters of the second order rate equation. Each of the measured optical densities was given a weight of 1.00. The program could simultaneously determine variations in as many as six parameters. These parameters were the initial chromium(II) and chlorate ion concentrations, initial and final optical densities, zero time error and the second order rate

---

*The authors wish to acknowledge the generous assistance of Dr. T. W. Newton and Dr. Roger Moore for making the Los Alamos program available. A detailed description of the program appears in the Los Alamos publication LA-2367.

constant, k_1. The most pertinent output data included an estimated standard deviation for each of the parameters and a comparison of the observed and calculated optical density and its standard deviation at each time t. Several different combinations of parameters to be estimated were chosen; in each case, the variations in these parameters were less than the known accuracy of the parameter itself. In each case, the final values of k_1 were identical within the limits of one standard deviation.

It should be emphasized that the computer programs provide an empirical fit for the input data. However, essentially identical values are obtained whether the linear or the nonlinear least squares program is used.* Therefore, the nonlinear program with unit weights for each datum point was used.

Experimental Test of the Kinetic Calculations: For the computations, it was tacitly assumed that the distribution of the chromium(III) products is the same throughout the course of the reaction. If this assumption is correct, the value of the rate constant should be independent of the wavelength used to follow the reaction even though the ratios of the extinction coefficients of the chromium(III) products might vary markedly. The assumption was tested experimentally by repeating the same kinetic run at 4100 Å, 4800 Å, 5400 Å, and 5800 Å. The values of the rate constants obtained are the same within the precision of the experiments at each wavelength, although the ratios of the extinction coefficients for the three products vary considerably over this wavelength range.

(4) High temperature spectra of aqueous solutions

During the last year, experimental work has been concentrated on the recording of high temperature spectra. Measurements have been made up to 110°, but due to poor optical and electronic performance of the spectrophotometer, these are of doubtful accuracy. However, these defects in instrumentation appear to have been corrected, and final results should soon be forthcoming.

Originally, high temperature spectra were taken by heating the compartment with water from a constant temperature bath. Since this heats the entire compartment, some heat leaks into

---

*For example with 2.17×10^{-2} M Cr(II) and 3.28×10^{-3} M ClO_3^- the k_1 values for the linear and nonlinear program were 38.7 ± 1.2 and 38.5 ± 1.0 at 5800 Å and 39.3 ± 1.0 and 38.9 ± 0.6 at 4500 Å respectively.

the monochromoter compartment, which causes a discrepancy between the read and the indicated wavelength. The cell was therefore heated directly by means of a heating wire.

Since water is the sample, it is not possible to use a reference cell filled with water. Therefore, the reflectances of the cell windows must be taken into account by other means. We have measured these reflectances by several methods. However, the easiest and most accurate way is to fill the cell with CCl_4, which has a low absorbance in this region and has about the same refractive index as the cell material, so that the outside reflectances and the absorbances of the cell are automatically accounted for. The only additional corrections necessary are for the absorbance of 1 cm. CCl_4 (-0.003) and the water-cell interface reflection (+0.002). By pressurization this cell can be heated to 90° so that the zero line can be established under approximately the same conditions as the actual experiments.

A nonlinear least squares program has been adapted for analysis of the data. The fit obtained at the central portion of the curve for 25° (8850-8130 $cm.^{-1}$) has been improved to where the sum of the squares of the deviations is $\sim 7 \times 10^{-4}$ for all points. When the entire curve is used (measured from the minimums on both sides - 9346-7937 $cm.^{-1}$), the sum of the squares of the deviations is somewhat poorer. This is due to the presence of interfering bands at the wings, which cause the calculated absorbance to be much less than the measured. In order to separate the effects of the interfering neighboring bands from the effects of the librational satellites, the baseline was raised to the minimum at 9346 $cm.^{-1}$. The sum of the squares of the deviations remained very nearly the same, and the existence of the librational satellite (or satellites) appeared to be confirmed.

(E) Programming systems for numerical analysis

(1) Program review for SHARE's numerical analysis project

Principal investigator

Dr. Richard H. Austing	Assistant Professor	Computer Science Center

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
001/63/018	9/63	6/65	0/8	2/22
001/65/037	3/65	In progress	3/35	3/35

The program to test eigenvalue-eigenvector routines for real symmetric matrices is well under way and significant results have already been obtained. However, several routines recently have appeared in the literature which should be evaluated before final comparisons of the various methods are made. It is expected that modifications will have to be made in some of these routines before they can be run on the Center's system.

A comprehensive test plan has been devised. It has been applied to the following programs:

(a) SHARE #3132: Threshold Jacobi method.

(b) SHARE #3096: Givens-Householder method.

(c) Givens-Householder Method described in [1].

Additional Jacobi and Householder routines are still to be investigated. They are presently undergoing necessary programming modifications prior to inclusion in the test plan.

A large sampling of matrices of orders 2 through 32 was used in testing these programs. These matrices consisted of known test matrices and matrices with known eigenvalues and eigenvectors generated either from tensor products of smaller matrices or by the method of J. Ortega [2]. The following results have been obtained:

(1) (a) is generally the fastest of the three methods of obtaining all eigenvalues and eigenvectors of a real symmetric matrix of order ≤ 15 and (c) is the fastest method for orders > 15.

(2) (c) is up to four times faster than (b).

(3) All three methods give eigenvalues and eigenvectors of approximately the same degree of accuracy.

(4) Orthogonality of eigenvectors is more nearly achieved in (a) than in either (b) or (c).

On the basis of these results, there seems to be no reason to recommend (b) to a user.

Upon completion of the testing of additional routines, a detailed report will be produced and testing of another class of routines will be initiated. Results and recommendations contained in the report should eliminate a number of problems users encounter when relying on an untested routine. Also computer time will be saved through the use of properly tested, well documented, efficient programs.

References

1 J. Ortega, The Givens-Householder Method for the Symmetric Eigenvalue Problem, in A. Ralston and H. Wilf (Eds.), Mathematical Methods for Digital Computers, Vol. 2, in press.

2 J. Ortega, Generation of test matrices by similarity transformations, Comm. ACM, 7, 1964.

(2) An evaluation of the usefulness of FORMAC

Principal investigator

Mr. Howard D. Wactlar — Research Programmer — Computer Science Center

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
001/65/050	10/65	In progress	2/41	2/41

FORMAC [1] is now operational as part of an independent IBSYS system at this Center. No attempt has been made to check out the FORMAC processor, only to assure that our setup produces precisely the same results as IBM's on their distributed sample programs.

FORMAC does provide some interesting features for algebraic manipulation. In addition to its ability to perform arithmetic on expressions, it also provides partial differentiation. It recognizes such basic functions as sine, cosine, log, exp., atn., and htn., with expressions as arguments. It is quite easy to make the transition from programming in Fortran IV to programming in FORMAC, as the set of F IV statements may be regarded as a subset of FORMAC.

However, there are many disadvantages and limitations to the use of FORMAC:

1) FORMAC requires rather involved input/output operations. This is demonstrated by sample programs to perform second order differentiation. Of the 36 program statements, only 2 performed algebraic manipulations, 4 were declaration statements, and the remainder were I/O statements.

2) As with many list processors, FORMAC runs out of available core before it can be genuinely useful. Translated matrix inversion and determinant expansion examples [2,3] in which algebraic expressions were substituted for single variables, demonstrated this problem all too well. Successful results were limited

to 5 x 5 matrices of 25 independent elements. The FORMAC object-time subroutines may require as much as 16K storage in addition to the requirements of the main program. Storage requirements may be eased by segmenting a program into links and overlaying (chaining) them. One must proceed here with great caution, however, because of the black box nature of the FORMAC object-time routines.

3) Because FORMAC translates its program to Fortran IV and then compiles the F IV program, its total compilation time is relatively high. The execution time is greatly slowed by the interpretive execution of the FORMAC subroutines and the necessity to temporarily throw onto tape those expressions that are not being used in order to provide more working core.

To facilitate further experimentation with FORMAC, a matrix output routine and a clocktiming routine have been made available.

In summary, the performance of FORMAC is disappointing in its present state because its limitations are too restrictive for many research problems. FORMAC is merely a collection of macros or subroutines designed for performing a restricted set of operations. As a list processor and string manipulator it is in great need of those facilities which permit the building of pattern recognition functions. For example, FORMAC allows one to replace sin2u with 2sinucosu, but does not provide a reasonable facility for simplifying the latter expression to the former; the situation is worse for $\sin^2 u + \cos^2 u = 1$. The problems of programming FORMAC to integrate are immense, since it provides no building blocks.

References

(1) J. E. Sammet and E. R. Bond, IEEE Trans. Elec. Comp., EC-13 (August 1964) 386

(2) T. C. Wood, Algorithm 42, Comm. ACM 4(April 1961) 176; A. W. Knapp, R. Shaman, Cert. Alg. 42, Comm. ACM 4 (Nov. 1961) 498; P. Naur, Rev. Alg. 42, Comm. ACM 6 (January 1963) 38

(3) J. G. Solomon. Algorithm 41, Comm. ACM 4 (April 1961) 176 B. H. Freed, Rev. Alg. 41, Comm. ACM 6 (Sept. 1963) 520

(F) Computing system for chemical engineering problems

Principal investigator

Mr. Chan M. Park	Research Programmer	Computer Science Center

			Computer time*	
Project No.	Initiated	Completed	Reporting period	Total
001/64/019*	11/64	In progress	2/3	3/17

Publication (during reporting period):

Computer Science Center Technical Report TR-65-24, Subroutines for Digital Computation of Chemical Engineering Problems, Part I, by Chan M. Park, October, 1965

The report referenced above contains a collection of subroutine programs designed to aid chemical engineers in the solution of their problems. The routines are divided into two classes. Those in the first class are non-mathematical (unit conversion and plotting), while those in the second class are numerical analysis routines (interpolation, elimination, least squares fit, matrix multiplication and inversion, numerical integration, and solution of first order ordinary differential equations).

Additional routines dealing with ordinary and partial differential equations, as well as programs for solving specific chemical engineering problems involving kinetics, diffusion, and transport phenomena, are presently under development, and will be the subject of Part II of the above report.

List of subroutines already developed

Designation	Purpose
CONVRT	Unit conversion
LNPLOT	Log-log plot
LAGINT	Lagrangian interpolation
GAUSS	Gauss elimination
LEASQU	Least-squares fit
MATMPY	Matrix multiplication
MATINV	Matrix inversion
SIMPSN	Numerical integration by Simpson's method
RUNMOD	Modified Runge-Kutta Method

*In the time summaries of Appendices 1-2, computer time used on this project is included under the College of Arts and Sciences

(G) Statistical computing systems

(1) Development and testing of statistical programs

Principal investigator

Mr. James F. Williams	Research Programmer	Computer Science Center

			Computer time*	
Project No.	Initiated	Completed	Reporting period	Total
001/65/031	2/65	In progress	1/32	1/32

Work on a comprehensive item analysis computer program is nearing completion. The need for such a program develops in the process of constructing a test which significantly contributes to the prediction of a specified measure.

The particular case which immediately comes to mind is that of the classroom examination. More often than not, the examiner constructs tests by selecting items which are considered critical in the evaluation of examinee achievement; all items are assumed to contribute to an accurate measure of performance. Due to the examiner's faith in the validity of the components of his system, the adequacy of the test as a predictor is seldom questioned.

Even where the validity of the items is doubtful, the technique of item analysis is extremely time-consuming. In general, the task is to select from a test or sub-test those items which discriminate between two criterion groups and to reject those which fail to do so, assuming that the test or sub-test measures a unitary factor and that the criterion itself is valid. The purpose here is to increase the validity of the test by including items which are positively correlated with the criterion and excluding those which have a negative or zero correlation with it. However, as the number of items and/or subjects becomes even moderately large, the task is as almost impossible one; the additional possibility of cross-validation can approximately double the work required. For these reasons, computer program to perform these operations would be a definite asset in the construction of predictors.

*The time used on this project prior to December 1965 is not included in Appendix 2.

Academic achievement evaluation, however, constitutes only a small part of predictor design; the more general problem of classification (including selection and placement) might also be attacked using the technique of item analysis. During the summer of 1965, an earlier version of the item analysis program was utilized to devise a job classification system for a branch of the armed forces. A questionnaire of 532 items was administered to approximately 15,000 men classified into 33 occupational groups. For each group, 25-50 of the most valid items were selected and given unit weights; those not selected were given zero weights. The total score of the original sample was correlated with an external criterion of a job performance rating; this procedure was repeated for the cross sample. The result of this study was that the items selected did not significantly contribute to an adequate classification system. However, the point worth stressing here is that this result only became manifest after cross-validation, this feature being one of the more important aspects of the present computer program. Unless cross-validation is included as a part of the project, the results can often be misleading.

In summary, this program was designed to facilitate analysis of test items and to aid in the construction of more valid predictors.

(2) Programs for statistical analysis

Principal investigators

Dr. Nancy S. Anderson	Associate Professor Research Consultant	Psychology Computer Science Center
Dr. Leopold O. Walder	Associate Professor Research Consultant	Psychology Computer Science Center

Project No.	Title	Initiated	Completed	Computer time Reporting period	Total
206/63/008	Evaluation of BIMD and ANOVA programs	1/64	In progress	0/24	6/10
206/63/009	Programs for statistical analysis	9/63	In progress Reactivated	0/23	4/38

The time used on the above two projects since September 1965 has been credited to the College of Arts and Sciences in Appendices 1-2.

206/64/006	Development of programs for statistical and psychological research	2/64	In progress Reactivated	1/50	1/50

The time used on this project prior to September 1965 is not included in Appendix 2.

(H) Management information structures

Principal investigator

Mr. Zalman A. Shavell	Research Programmer	Computer Science Center

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
001/66/055	1/66	3/66	0/8	0/8

To date, this project has sought to determine the required inputs to the USAF-PERT COST system and is at a stage where computations with test networks may be attempted. A corollary investigation into the problems associated with a real-time PERT-TIME system has been made and some preliminary programs in this area are currently in preparation.

However, most of the work on this project must be suspended because the principal investigator has been called to active duty with the U. S. Air Force.

2. Computer and information sciences research

(A) Numerical analysis

(1) Numerical solution of non-linear operator equations

Principal investigators

Dr. Werner C. Rheinboldt — Research Professor

Dr. James M. Ortega — Research Assistant Professor

Computer Science Center and Institute for Fluid Dynamics and Applied Mathematics

In cooperation with

Mr. James Vandergraft — Research Associate — Computer Science Center

Project No.	Title	Initiated	Completed	Computer time: Reporting period	Computer time: Total
001/64/013	Numerical solution of non-linear functional equations	7/64	In progress	13/4	19/17
001/64/015	Relaxation techniques in the solution of certain boundary value problems	7/64	6/65	3/38	5/32
001/65/042	Experiments with minimi-zation techniques in numerical analysis	6/65	In progress	1/28	1/28

Publications (during reporting period):

W. C. Rheinboldt, On a General Estimation Principle and a Theory of Comparison Factors, Technical Report TR-65-14, March 1965

J. M. Ortega and W. C. Rheinboldt, On Discretization and Differentiation of Operators with Application to Newton's Method, Technical Report TR-65-16, May 1965; accepted for Publication in SIAM Journal of Numerical Analysis

J. M. Ortega and M. L. Rockoff, Non-linear Difference Equations and Gauss-Seidel Type Iterative Methods, Technical Report TR-65-20, August 1965

Five areas of current research under this project are

(a) A general rigorous study of the definition, generation and analysis of iterative processes.

(b) Study of particular classes of iterative processes that reduce to known iterative processes for systems of linear algebraic equations. Such processes will be called generalized linear processes.

(c) Study of various aspects of Newton's method and, in particular, monotonic behavior of the iterates produced by Newton's method when the underlying space is a vector lattice.

(d) Study of imbedding techniques for extending the domain of convergence of a given iterative process.

(e) Compilation of a comprehensive survey of the literature on iterative processes and of a bibliography.

Considerable progress has been made in the general study of relaxation methods for non-linear equations. In two areas, reports are currently in preparation.

(a) Approximate iterations

For the numerical solution of a non-linear system of equations, one interesting relaxation method is derived as follows: Apply Newton's method; this requires solving a sequence of linear problems. If one is dealing with the discrete analogue of, for example, a partial differential equation the solution of these linear problems will also require an iterative procedure. Consider the application of the Gauss-Seidel procedure in the following way. At the kth Newton iteration, take precisely k Gauss-Seidel iterative steps toward solution of the linear system. This leads to an iteration of the form (1) $x_{m+1} = F_m x_m$, where F_m is an iteration operator whose form is

a function of m. Ehrmann [1] had previously studied iterations of the form (1) in an abstract setting, and it has been possible to apply his results to this problem. Schmidt [2] has also considered a similar abstract problem, namely iterations of the form $x_m = F_m x_m$ - that is, the x_m are themselves solutions of fixed point equations. Related to this, but arising from entirely different considerations in the theory of rounding error, are results of Ostrowski [3] and Urabe [4]. Motivated by these seeming, and previously undetected, similarities, these various theories have been combined so that the underlying principles have become apparent. This investigation has been conducted primarily in the setting of R^n - metric spaces -- that is, spaces metricized by elements of real Euclidean space. This is suitably general not only for the original questions but for a wide variety of applications. More generally, with Ehrmann and Schmidt, extensions to more general spaces metricized by elements of a partially ordered topological linear space have been considered. Not all of the results extend, and this gives rise to several interesting topological and analytical questions, some of which are currently being investigated. A full report on this work is in preparation.

(b) Monotone convergence of Gauss-Seidel Methods

A recent paper of considerable interest, by Greenspan and Parter [5], has motivated the study of the monotonic behavior of iterates produced by Gauss-Seidel methods. It has been discovered that the results of Greenspan and Parter were largely anticipated by two Russian mathematicians, Baluev [6] and Slugin [7], who studied similar monotonicity questions in abstract spaces. It has been possible to extend some of these results to implicit Gauss-Seidel processes and also to clarify and encompass the work of Greenspan and Parter. An attempt is now being made to extend this to successive over-relaxation methods; here the setting is somewhat more difficult. A report on this work is in the early stages of preparation.

(c) Monotonic convergence of Newton's method

Mr. Vandergraft's work on the monotonic behavior of Newton iterates on a partially-ordered linear topological space is nearing completion. Some rather general theorems have been found which guarantee that Newton's method applied to certain types of convex operators will produce a monotone sequence which converges to a zero of the operator. If the operator has a continuous Frechet derivative, the convergence is shown to be superlinear; if the second Frechet derivative is also continuous, then quadratic convergence results. These

theorems cover the equations considered by Kalaba as well as those of Parter and Greenspan. Moreover, a theorem of Kantorovich, concerning the convergence of Newton's method for general operators, is contained in these results, as are some theorems of Baluev for Chaplygin type approximations.

(d) Invariant imbedding

A graduate research assistant, Mr. G. Meyer, is investigating the theoretical foundation of the so-called method of invariant imbedding. This method is of great importance in many applications of transport theory and concerns the solution of special boundary value problems for ordinary differential operators, integro-differential operators, as well as partial differential operators. It has been found that the central idea of the method can be interpreted in the context of the theory of characteristics for partial differential equations of the first order. This leads to the possibility of obtaining theoretical results on the existence and uniqueness of the solutions and of connecting the method with the theory of initial value problems for first order partial differential operators. A generalization of the theory of characteristics to operators on Banach spaces opens up interesting possibilities for solving transport problems involving boundary value problems for systems of first order partial differential equations.

(e) Mildly non-linear elliptic equations

A NASA trainee, Mr. R. Elkin, is currently investigating several questions arising in the numerical solution of elliptic boundary problems of the form $\Delta u = f(u, u_x, u_y)$ with Dirichlet boundary conditions. In particular, he is trying to extend some of the previous results on the asymptotic rate of convergence of Gauss-Seidel iterative methods as well as to apply results of Baluev mentioned previously in order to guarantee monotonic convergence.

References

[1] Ehrmann, H., Iterationsverfahren mit veraenderlichen Operatoren, Arch. Rat. Mech. Anal., 4, 1, 1959, 45-64

[2] Schmidt, J., Konvergenzuntersuchungen und Fehlerabschaetzungen fuer ein verallgemeinertes Iterationsverfahren., Arch. Rat. Mech. Anal., 6,4, 1960, 261-276

[3] Ostrowski, A., The Rounding-Off Stability of Iterations, Basel Mathem. Notes, BMN-12, August 20, 1964

[4] Urabe, M., Error Estimation in Numerical Solution of Equations by Iteration Processes, J. Sci. Hiroshima Univ., A-I, 26, 1962, 77-91

[5] Greenspan, D. and S. Parter, Mildly Non-linear Elliptic Partial Differential Equations and Their Numerical Solution II, MRC Techn. Report #474, May 1964

[6] Baluev, A. N., On the Method of Chaplygin (Russian) Vestnik Leningrad, 13, 1956, 27-42

[7] Slugin, S. N., Approximate Solution of Operator Equations by the Method of Chaplygin, Doklady, 103, 1955, 565-568

(2) Nonlinear oscillations and integral equations

Principal investigator

Dr. Abraham Tal — Visiting Research Assistant Professor — Computer Science Center

(a) Nonlinear eigenvalue problems

The nonlinear differential equation

$$y' + yF(y, \lambda, x) = f(x) \tag{1}$$

with the boundary conditions

$$\alpha y(a) + \beta y(b) = 0 \qquad \alpha y(a) + \beta y'(a) = 0$$

or

$$\gamma y'(a) + \delta y'(b) = 0 \qquad \gamma y(b) + \delta y'(b) = 0 \tag{2}$$

is a generalization of Duffing's Equation and has many applications in the theory of nonlinear oscillations [1].

Under suitable conditions (1) + (2) possesses an eigenvalue and a corresponding eigensolution, this latter having a prescribed number of zeros in (a,b).

Theoretical investigations have indicated that a two-dimensional version of Newton's Method [2] may be adequate to the numerical treatment of this equation.

It is proposed to undertake the examination of this particular problem as well as its possible generalizations to other nonlinear eigenvalue problems.

References

[1] A. Tal, On a Class of Nonlinear Eigenvalue Problems, Thesis, C. I. T., Pittsburgh 1965.

[2] L. Collatz, Funktionalanalysis und Numerische Mathematik, Springer, Berlin 1964.

(b) Integral equations of the first kind

As described in the previous status report, Fredholm's equation of the first kind

$$\int_a^b k(x,t)f(t)dt = g(t)$$

yields highly oscillating solutions when finite difference discretization is employed.

Among the various alternatives to this approach two processes have been found to be more or less satisfactory:

a) The method of steepest descent [1]

b) The conjugate gradient method [2]

Solutions obtained by these methods are stable, but their accuracy is relatively low - within 1-3% - due to the slow convergence of the iterations involved.

A third method - based on optimal approximation [3] - is currently under examination. It is hoped to modify it in such a way as to yield that solution of (1) which is most significant for the particular problem in consideration.

References

[1] L. V. Kantorovich, Functional Analysis in Normed Spaces, Macmillan 1964.

[2] M. R. Hestenes and E. Stiefel, Methods of Conjugate Gradients for Solving Linear Systems, J. Res. Nat. Bur. Standards, V. 49, p. 409, 1952.

[3] M. Golomb and H. F. Weinberger, Optimal Approximation and Error Bounds, On Numerical Approximations, R. E. Langer, ed., pp. 117-190, Madison, Wisconsin, 1959.

(3) Eigenvalue approximation

Principal investigator

Dr. John E. Osborn Assistant Professor Mathematics

Let L be an unbounded self-adjoint operator whose inverse is a Hilbert-Schmidt operator on a Hilbert space. Let A be a linear operator defined on the domain of L which is not assumed to be self-adjoint but is assumed to be small relative to L in the sense that either:

(a) A is bounded, or

(b) A is a differential operator of order p and L is a differential operator of order q where $p < q$.

Assuming that the eigenvalues and eigenvectors of L are known we consider the problem of approximating the eigenvalues of $\tilde{L} \equiv L+A$. These eigenvalues will in general be complex, so it is desired to find regions of the complex plane which contain some or all of these eigenvalues. It is also desired that the estimates obtained be computable. For case (a) a method for approximating the eigenvalues of $\tilde{L}$ is given in [3]. Procedures for approximating the eigenvalues of classes of nonself-adjoint operators different from that outlined above are presented in [1,2].

It is planned to investigate the following areas which are related to the problem formulated above:

(1) Extension of the results of [3] to case (b). This would give a procedure for approximating the eigenvalues of certain nonself-adjoint differential operators.

(2) For case (a), removal of the restriction of [3] that the eigenvalues of $\tilde{L}$ be simple. This would allow the approximation of multiple eigenvalues of $\tilde{L}$.

It is also proposed to undertake a program of numerical computation designed to illustrate and test the methods of [3] and any methods obtained under (1) and (2) above by considering examples of interest in applied mathematics.

References

1. Fichera, G., "Su un metodo del Picone per il calcolo degli autovalori e degli autosoluzioni," Ann. Mat. Pura. Appl., Ser. 4, Vol. 40 (1955), pp. 239-259.

2. Mysovskih, I. P., "On an estimate of the error in eigenvalues calculated by replacing the kernel by another close to it," Mat. Sb. (N.S.) 49(91) (1959), pp. 331-340.

3. Osborn, J. E., "Approximation of the eigenvalues of non-self-adjoint operators", Technical report, University of Minnesota, 1965. (Submitted to J. Math. and Phys.)

(4) Numerical solution of differential equations by collocation methods

Principal investigator

Dr. John Mason	Research Associate	Institute for Fluid Dynamics and Applied Mathematics

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
303/65/016	9/65	In progress	3/45	3/45

Publications (during reporting period):

Institute for Fluid Dynamics and Applied Mathematics Technical Notes, BN-428, Chebyshev polynomial approximations for the L-membrane eigenvalue problem;

BN-430, Approximate formulae for a variety of solutions of the Thomas-Fermi equation

The project is a continuation of work done at Oxford University in a D. Phil. thesis. The standard Chebyshev collocation methods involve polynomial approximations and ordinary differential equations. The aim of this project has been to generalize these methods to rational approximations and partial differential equations.

The methods produce systems of linear or non-linear simultaneous algebraic equations. Part of the project is therefore concerned with finding methods for solving these systems efficiently. Previous programs have been based on Newton's method.

The immediate aim is to complete computations begun at Oxford for two specific problems connected with the project. One of these relates to general solutions of the Thomas-Fermi equation, while the other is on the eigenvalue problem for a vibrating L-shaped membrane.

References

[1] Lieberstein, H. M., A continuous method in numerical analysis applied to examples from a new class of boundary value problems, M. R. C. Technical Summary Report 175, University of Wisconsin, 1960.

[2] March, N. H., Thomas-Fermi fields for molecules with tetrahedral and octahedral symmetry, Proc. Camb. Phil. Soc. 48, 665, 1952.

[3] Mason, J. C., Rational approximations to the ordinary T.-F. function and its derivative, Proc. Phys. Soc. 84, 357, 1964.

[4] Mason, J. C., Some new approximations for the solution of differential equations, D. Phil. thesis, Oxford, 1965.

(5) Numerical integration

Principal investigator

Mr. Charles K. Mesztenyi	Senior Research Programmer	Computer Science Center

In cooperation with

Dr. Seymour Haber, National Bureau of Standards

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/65/046	Multiple quadratures	6/65	In progress	4/42	4/42

(6) Approximation of functions

Principal investigator

Mr. Charles K. Mesztenyi	Senior Research Programmer	Computer Science Center

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/63/015	Chebyshev approximations for elementary and special functions	7/63	In progress (reactivated)	12/2	37/35
001/65/039	Orthogonal polynomials over discrete ranges and applications	4/65	In progress	2/39	2/39

(7) An inhomogeneous singular problem for the equation of Euler-Poisson-Darboux

Principal investigator

Mr. B. A. Fusaro	Instructor	Mathematics

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
203/65/012	2/65	3/65	0	0/4

(B) Image processing

(1) Digital image processing techniques

Principal investigators

Dr. Azriel Rosenfeld	Research Associate Professor	Computer Science Center
Mr. John L. Pfaltz	Senior Research Programmer	Computer Science Center

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/64/020	FRAME - A study of circumscribed rectangles that "frame" a shape	11/64	6/65	0/2	6/52
001/64/022	RAMP - Region area measurement program	12/64	In progress	2/2	4/10
001/64/023	Analysis and thinning of locally "pseudo one-dimensional" shapes	12/64	5/65	0	0/41
001/64/026	Development of utility routines for image processing procedures	12/64	In progress	11/18	13/56
001/64/027	Generation and analysis of shape skeletons	12/64	In progress	5/58	7/17
001/65/038	Study of graphs as related to image processing	4/65	10/65	2/52	2/52

Publications (during reporting period):

Image Processing, A. Rosenfeld, Proc. 3rd Ann. Conf. on Urban Planning Info. Systs. and Programs (1965), 49-52

Sequential Operations in Digital Picture Processing, A. Rosenfeld and J. L. Pfaltz, Jour. ACM 13 (1966), in press

The programs for region connectivity and "propagation" described in earlier reports have been rewritten for application to hexagonal (rather than rectangular) arrays of points. This has the advantage that the connectivity "paradoxes" (failure of the Jordan Curve Theorem) which hold for rectangular arrays do not arise in the case of a hexagonal array. In addition, the "propagation" process is appreciably more nearly Euclidean in a hexagonal array, where neighborhoods are hexagonal rather than square.

Preliminary work has been done on the application of thresholded "propagation" processes to cluster detection. Studies of "framing" shapes with rectangles, and of detecting curvature maxima in the boundary of a shape, have been discontinued due to the pressure of more urgent work.

(2) Cloud pattern analysis

Principal investigator

Dr. Azriel Rosenfeld	Research Associate Professor	Computer Science Center

In cooperation with

Mr. James N. Orton	Electronic Data Processing System Analyst	Budd Information Sciences Center

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/65/036	SORD - Computer programs for subdividing an image into "solid" and "broken" regions	3/65	In progress	29/13	29/13

Publications (during reporting period):

Automatic Cloud Interpretation, A. Rosenfeld, C. Fried and J. N. Orton, Photogram. Eng. 31 (1965), 991-1002.

This research is a cooperative effort of the Budd Information Sciences Center, McLean, Va., and the Computer Science Center. The Budd portion of the work was supported by Contract NAS5-9551 between the Budd Company and NASA's Goddard Space Flight Center. A Final Report on this Contract, dated January 31, 1966, was recently submitted to NASA. This report includes descriptions of the SORD and BRAND programs for discriminating "solid" from "broken" regions in an image and classifying the latter according to "degree of brokenness". These programs have been generalized to apply to digitized pictures containing up to fifteen gray levels. As a useful by-product, a local brokenness test has been used to detect picture elements at which the density gradient is high.

(3) Bubble chamber film analysis

Principal investigator

Dr. Robert Glasser	Associate Professor	Physics and Computer Science Center

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
203/65/014	Simulation of pattern recognition of particle tracks in bubble chamber films	7/65	In progress	3/16	3/16

This project is temporarily inactive. Preliminary results indicate the feasibility of simulating the operation of a PEPR processor on simple tracks with relatively little background under conditions in which it was possible to store a complete description of the section of the picture under consideration in the machine memory. The time required was of the order of 100 times slower than would have been required by a real PEPR. This should be regarded as an encouraging indication. The main residual problem is to find a sufficiently efficient method of buffering data in those cases (which form the dominant interesting category) in which it is necessary to store most of the data on auxiliary storage.

(4) Map analysis and output

Principal investigators

Dr. Azriel Rosenfeld	Research Associate Professor	Computer Science Center
Mr. John L. Pfaltz	Senior Research Programmer	Computer Science Center
Mr. Mark S. Monmonier	Graduate Research Assistant	Computer Science Center

In cooperation with

Dr. Allen A. Schmieder	Assistant Professor	Geography

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/64/021	SAMP-Surface area measurement program	11/64	10/65	12/15	15/48
353/65/002	Spatial shading picture	3/65	8/65	0/5	0/5
353/65/003	Automated shaded map	4/65	8/65	0/4	0/4

Publications (during reporting period):

SAMP - A Computer Program for Estimating Surface Area from Contour Maps, M. S. Monmonier, J. L. Pfaltz and A. Rosenfeld, Computer Science Center Technical Report TR-65-21, August 1965; Photogram. Eng. 32 (1966), in press.

The Production of Shaded Maps on the Digital Computer, M. S. Monmonier, Professional Geographer 17 No. 5 (1965), 13-14

(C) Visual perception and pattern recognition

Principal investigators

Dr. Nancy S. Anderson	Associate Professor Research Consultant	Psychology Computer Science Center
Dr. Azriel Rosenfeld	Research Associate Professor	Computer Science Center

Studies are being conducted to determine the dimensionality and scale distances used by subjects in the judgment of statistical stimulus patterns. The ultimate objective is to investigate the characteristic, "salient" features used by subjects to discriminate and classify abstract visual textures or patterns. The particular patterns for this series of studies are 10x10 matrices of line segments differing in angle of orientation. Eight different orientations are used, varying from 0 degrees to 157.5 degrees in equal steps of 22.5 degrees.

Subjects are shown a sample of 1) a "random" pattern, in which lines at all eight orientations appear equally often and 2) a structured pattern, one in which one particular orientation occurs with a probability of approximately 0.9. Ss then make several scaling judgments of all or selected possible pairs of patterns, using the psychophysical method of successive intervals. Essentially, this method requires Ss to judge on a 1 to 7 scale the similarity of a pair of the statistical patterns. (The 1 to 7 scale ranges from 1 = most similar to 7 = very different.) The method of successive intervals is used in order to allow an evaluation of the multi-dimensionality of stimulus judgments.

Although the present statistical patterns used for the preliminary study vary only with respect to how frequently one given orientation occurs, future studies will employ patterns in which arbitrary frequency distributions of the different orientations will be used.

Preliminary data indicate that subjects are reliable in their judgments about the similarity of or differences in pairs of patterns, and that there is agreement between subjects on the scale values chosen for the different pairs of patterns.

With the data that are being collected, and using these scaling techniques, it should be possible to determine from the judgments what is the minimum dimensionality of the stimulus set and what are the scale values (projections on the dimensions) for each of the statistical textures used. These determinations of the projections on axes of a Euclidean Space are calculated from the interpoint distances between all pairs of patterns. From these data it should be possible to determine what features subjects use to discriminate various kinds of non-randomness in textured patterns. The features will be helpful in devising models which specify how people discriminate textures.

(D) Procedure languages and system structures

(1) ALGOL

Principal investigator

Dr. Earl J. Schweppe	Associate Professor	Computer Science

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/63/017	Programming language usage study	9/63	In progress	0/57	36/53
001/65/035	ALCOR-Illinois 7090/94 compiler for ALGOL 60	3/65	In progress	3/22	3/22

Work with the ALCOR-Illinois 7090/94 Compiler for ALGOL 60 is continuing. Numerous corrections to the compiler have been received recently and are in the process of being incorporated into the system. It is hoped that these modifications will correct most of the discrepancies which we have reported to the developers. After making these modifications, extensive testing of the compiler will be carried out once again. Most of the other activities in connection with this compiler are being held in abeyance until the compiler has been up-dated. The U of M 1401 transliteration preprocessor for ALGOL 60 to ALCOR-Illinois 7090/94 is no longer usable, since the Center relinquished its Flexowriter. This preprocessor may be redeveloped for the System 360 to take advantage of the extended character set available on that machine.

(2) Consequent procedures

Principal investigator

Dr. Earl J. Schweppe	Associate Professor	Computer Science Center

In cooperation with

Dr. D. R. Fitzwater, Institute for Atomic Research and Department of Chemistry, Iowa State University, Ames, Iowa

Project No.	Title	Initiated	Completed	Computer time Reporting period	Computer time Total
001/65/034	Simulation of consequent procedure system task structures	3/65	In progress	0/1	0/1

Work on this project is proceeding somewhat slowly; however, it is hoped that a revised version of the more theoretical paper entitled "Consequent Procedure Networks" can be completed during the next six months.

(3) Tree structure processing

Principal investigator

Dr. Earl J. Schweppe	Associate Professor	Computer Science Center

Project No.	Title	Initiated	Terminated	Computer time Reporting period	Computer time Total
001/65/033	System for macro indexing and looping in tree structures (SMILTS)	3/65	2/66	0	0

For a variety of reasons, work on this project has been discontinued. These reasons include the following:

a. Programming support has not been available because of the pressure of more urgent work.

b. Difficulties have been encountered with the macro generation facilities of the IBMAP assembler. Although these discrepancies have been brought to the attention of IBM, we have no indication that they will be corrected soon. It has been decided that the other available assemblers are not widely enough used to make the development of this system within them worthwhile.

c. Delays caused by a. and b. have made it untimely to continue work in this area on the 7094. Similar work may be carried out in the future on System 360.

(4) Multiple path, non-predictive, syntactive recognizer for implementing various ALGOL-like languages

Principal investigators

Dr. David L. Parnas	Assistant Professor	Computer Science* Center
Mr. Howard D. Wactlar	Research Programmer	Computer Science Center

Project No.	Initiated	Completed	Computer time Reporting period	Total
001/65/053	12/65	In progress	1/21	1/21

An ALGOL program has been written to accept a modified Backus normal form grammar, organize it, and store it in an easily manipulated internal form. The program will now be used for testing certain formal procedures for manipulating such grammars.

During the program development and testing stages a curious discrepancy in the ALGOL 60 Revised Report (1) and the ALCOR translator (2,3) was uncovered. Section 4.6.4.2 of the Report describes the execution of the "step-until" element in an unnatural manner, requiring two evaluations of the step element for each execution of the loop. The ALCOR translator in use at this Center adheres to what one assumes to be the otherwise intended meaning but still introduces another possible error resulting from its internal structure. These discrepancies have been reported to the Communications of the ACM.

References

1. P. Naur, et.al., Comm. ACM 6 (1963), 1-17.

2. D. Gries, M. Paul and H. R. Wiehle, Some techniques used in the ALCOR ILLINOIS 7090, Comm. ACM 8 (1965), 496-500.

3. R. Bayer, E. Murphee, Jr. and D. Gries, User's manual for the ALCOR ILLINOIS 7090 ALGOL 60 translator, 2nd. ed., U. of Illinois, 1964.

*Through January 1966

(E) The application of visual display man-machine interaction to nuclear optical model elastic scattering analysis

Principal investigator

Mr. Howard D. Wactlar	Research Programmer	Computer Science Center

Preliminary work on the above project has proceeded along three directions while awaiting the arrival of the required hardware configuration. First, simplified programming implementation techniques for graphical processing have been investigated. The two systems that have been studied are the MAGIC and MOBIDIC computers at the National Bureau of Standards and the Computer Aided Design program at Project MAC and M. I. T. A second, closely related investigation has been that of a proposed general purpose picture processing language for the IBM/360-2250 display configuration. Finally, an investigation has been conducted to evaluate and determine for the purpose of this specific project the best operating numerical and automatic parameter searching procedures in elastic scattering analysis.

(A) Program implementation techniques

MAGIC [1] is a custom built machine for graphical man-machine interaction possessing its own processing units independent of the main frame of another computer. It is in the process of being placed in a time-shared configuration with the MOBIDIC computer, also at the National Bureau of Standards. This hardware organization would be very advantageous for solving the problem being investigated on this project, since it would allow the high speed MOBIDIC processors to perform the optical model calculations while the MAGIC processor is determining and altering the details of the display and determining the points of interaction with user input. Although many of the implementation techniques used in the MAGIC system are strictly based upon the restrictions imposed by hardware design, some concerning its drum memory have proved to be worth considering. For example, the expansion, contraction and translation algorithms provide useful analogs for core memory manipulation of graphical data parameters.

The Computer Aided design program [2] which produced Sketchpad [3] and several derivatives provides a more basic underlying structure for graphical I/O implementation. At this time, the "plex" structure introduced by Ross and Rodriguez [4] seems to provide a favorable method worth building upon and implementing for this project on the IBM/360. Programming work in this direction has been initiated in advance of delivery of the IBM/360 Model 30 to the Computer Science Center.

(B) A proposed picture processing language

Discussions with other groups at this Center [5] concerned with graphical input/output have demonstrated the need for a generalized picture processing language that can be useful for both picture synthesis (this project) and analysis (pattern recognition projects). The premise is that a language which "describes" pictures is adaptable to both problems. A good internal structure for such a language is the plex structure already mentioned. Although Ross and Sutherland [3] have utilized it effectively for the representation of lines, its modeling is such as to allow its extension to other forms of data. If one interprets picture synthesis as producing a pattern from a given pattern and a modified set of parameters, while interpreting picture analysis as matching a given pattern with a given set of parameters to another pattern with a modified set of parameters, then one can design a language with the external structure of SNOBOL [6]. Substituting pattern descriptors for alphanumeric strings as data in a SNOBOL-like language tends to provide an easily implemented language upon which to expand for the needs of specific projects.

(C) Elastic scattering optical model analysis techniques

Work independent of reliance upon graphical input/output has been continuing on the IBM 7094 in order to determine optimum calculation and search techniques for optical model parameter fitting for elastic scattering experiments. A new program, SEEK [7], has been written based upon a modified version of the former SCAT4 [8] programs presently in use for such analysis.

The new program, which has undergone further modifications under this project, can compute cross sections, polarizations, and chi square deviations at a number of grid points for the

optical model parameters. It also possesses the ability to perform automatic searches over some of these parameters to find those sets of parameters which yield the best fits to the experimental cross sections and polarizations. If the theoretical reaction cross section at the best fit is not within the experimental uncertainties, the program commences a sequence of automatic searches for minimum chi square points, successively increasing (or decreasing) the values of reaction cross sections by a small amount, until the whole region of experimental uncertainties is covered. However, no further criteria are presently defined to determine which set of parameters from the collection of those representing the values within the experimental range is the best.

Using the data for p-Pb at 30.8 Mev [9] with 67 data points for cross sections and 21 for polarizations, and searching over 8 model parameters, the IBM 7094 required 1.9 minutes for an initial determination of the cross sections and polarizations and 4.8 minutes more to calculate results for 7 additional reaction cross section values in order to cover the entire experimental range with meaningful increments. The searching and analysis techniques applied here [10] provide an improvement by a factor of almost ½ in computer time over the ABACUS [11] program more commonly used for the search technique analysis. Many of the procedures applied in the current SEEK program will be expanded and utilized in this project, forming the calculational basis for the solution of our problem.

References

[1] Rippey, D. E., "MAGIC - A Machine for Automatic Graphics Interface to a Computer", National Bureau of Standards Report 8665, Dec. 1964.

[2] Coons, S. A. et al, An Outline of the Requirements for a Computer-Aided Design System" and related papers, Proc. Spring Joint Computer Conf., Detroit, Michigan, May 1963, pp. 299-353.

[3] Sutherland, I. E., "Sketchpad: A Man-Machine Graphical Communication System", Lincoln Laboratory Technical Report 296, Jan. 1963.

[4] Ross, D. T. and Rodriguez, J. E., "Theoretical Foundations for the Computer Aided Design System", Proc. Spring Joint Computer Conf., Detroit, Mich., May 1963, pp. 305-322.

[5] Parnas, D. L., private communication.

[6] Farber, D. J., R. E. Griswold, I. P. Polansky, "SNOBOL, A String Manipulation Language", Jour. Assoc. Comp. Mach., Vol. 11, p. 21, Jan. 1964.

[7] Melkanoff, M. A., T. Sawada, J. Raynal, "A FORTRAN Program SEEK for Automatic Searches for Elastic Scattering Analyses with the Nuclear Optical Model", unpublished communication.

[8] Melkanoff, M. A., T. S. Nodvik, D. S. Saxon, D. G. Cantor, "A FORTRAN Program for Elastic Scattering Analyses with the Nuclear Optical Model", Univ. of Calif. Press, Los Angeles, 1961.

[9] Melkanoff, M. A., J. Raynal, T. Sawada, "Nuclear Optical Model Calculations", to be published in Vol. V of "Methods in Computational Physics", edited by B. Adler, S. Fernbach and M. Rotenberg, Academic Press, New York and London, 1965.

[10] Devins, D. W., H. H. Forster and G. G. Gigas, Nucl. Phys. Vol. 35, p. 617, 1962; Craig, R. M., J. C. Dore, et al Nucl. Phys., Vol. 58, p. 515, 1964.

[11] Auerbach, E., Brookhaven National Laboratory, private communication.

(F) List processors and tree-structured data

Principal investigator

Mr. John L. Pfaltz — Senior Research Programmer — Computer Science Center

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
001/65/032*	2/65	10/65	9/0	9/21

The Symmetric List Processor documented by Weizenbaum in Comm. ACM, Sept. 1963 has been fully implemented in Fortran IV for use at the Computer Science Center. In the process, several corrections and additions were made to the published system. A complete user's manual for SLIP, together with a list processing primer, has been largely written and will be issued as a CSC Technical Report.

Since the use of any of the current list processors, including SLIP, requires a fairly detailed knowledge of list structures on the part of the programmer, a system called TREETRAN was written (see CSC Technical Report TR-65-23). While TREETRAN can only manipulate rooted trees, the user need have no knowledge of list structures and can perform a wide range of functions on tree structures with no more than a Fortran programming ability.

Two experimental problems involving geneological trees (bi-rooted trees) and generation of sentences from syntax tables were programmed using SLIP and TREETRAN respectively.

A system combining a number of picture processing and list processing concepts is now being developed. This system will simulate on-line interaction in the analysis of arbitrary two-dimensional images.

---

*Time used on this project is not included in Appendix 2.

(G) Experimental algebraic number theory

Principal investigator

Dr. Sigekatu Kuroda — Professor — Mathematics

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
203/63/002	3/63	In progress	11/51	59/53

Fundamental subroutines required for computations in algebraic number theory have been programmed for the IBM 7094. These programs have been assembled and preserved for future use in the form of over 1000 binary cards. They have also been preserved in the form of symbolic cards, totalling more than 20,000, to facilitate future changes and improvements. Both the binary and symbolic decks have been recorded on magnetic tape, and are available to other institutions upon request. The results of computations using these routines are also available on magnetic tape in binary or BCD form.

The subroutines mentioned above include one which in 10 to 125 seconds will store in core storage the prime number table for the interval n to n + 1,800,000 for any $n \leq 4 \times 10^9$. The latter bound can be extended up to a maximum of $2^{35}-1$. With this table, the primes belonging to any congruence group of class field theory can be generated, not only for the absolute case but also for some relative cases.

Also included are routines for computing number theoretic functions such as the Jacobi and Kronecker symbols and for finding primitive roots of primes. In addition, conversion programs from binary to duohexadecimal (duotricenary, i.e. base 32) and vice versa are included. The base 32 system is used because of the need to print out very large integers. A particular effort has been made to optimize the routines and establish printout formats.

Plans for the immediate future include

(1) Determination of the ideal class groups of real and imaginary quadratic number fields with prime discriminants, and distinguishing the very few cases of non-cyclic ideal

class groups.

(2) Determination of the ideal class groups of cyclic real biquadratic number fields with prime discriminants. This work was initiated during the summer of 1965 at the Technische Hochschule, Karlsruhe, Germany, with the cooperation of Professor H. W. Leopoldt.

Longer range plans for this project are as follows:

(1) Study of relative discriminants, Artin's L-functions, products of regulators and class numbers of the intermediate fields of a Galois extension of an algebraic number field of finite degree. This computation will employ the Artin-Brauer-Kuroda formula, using induced characters of the Galois group of the extension field.

(2) Extension of the results obtained on the structure of class groups to classes of relative extension fields for suitable choice of ground field (e.g., the Gauss field).

(3) Systematic investigations into the structure of ideal class groups and the decomposition laws of prime ideals in Galois extensions. These investigations should provide a basis for extending class field theory to the non-abelian case.

(4) Improvements in the computational programs, in particular so as to take advantage of the IBM/360 system to be installed at the Computer Science Center.

(H) Information storage and retrieval

Principal investigator

Dr. Howard E. Tompkins	Professor and Head	Electrical Engineering

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
305/64/006	7/64	In progress	7/9	15/25

A report on this project was not available in time for inclusion in this Report.

B. Computer-oriented research projects in other space-related fields

1. Molecular physics and spectroscopy

The sixteen projects in this section originate primarily in the Institute for Molecular Physics and the Department of Chemistry. (An exception is a doctoral dissertation project under the sponsorship of Professor Burgers of the Institute of Fluid Dynamics and Applied Mathematics.) One other project, involving collision integral calculations, was temporarily reactivated in July 1965; a detailed report on it was given in the Semiannual Status Report.

New projects

201/66/014	Spectroscopic studies of metal carbonyls
201/66/013	Rayleigh scattering of light
201/66/012	Calculation of solvent-solute interaction energy derivative terms
201/66/011	Studies of solute-solvent interactions
201/66/010	Thermodynamic constants for charge transfer complex formation reactions
202/66/008	Spectroscopic laboratory measurements and their relation to upper atmosphere observations
202/66/007	A study of the Brackett alpha emission of galactic nebulae
202/66/006	Determination of infrared line intensities, widths, and shapes
202/65/003	Intermolecular forces: The equation of state of dilute gases

Continuing projects

201/65/007	The evaluation of Franck-Condon factors for diatomic molecules
205/65/046	Shock tube measurement on relaxation time of hydrogen

202/64/002	Microwave spectroscopy studies
202/63/002	Computation of vibration-rotation matrix elements for diatomic molecules
202/63/008	Rydberg-Klein-Rees procedure for determination of alkali metal potential energy curves
202/63/006	Self-consistent field calculations

Completed projects

201/64/004	Vibrational calculations

(A) Spectroscopic studies of metal carbonyls

Principal investigator

Dr. Ellis R. Lippincott Professor Chemistry

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
201/66/014	1/66	In progress	0	0

Computational time is required for the solution of problems occurring in vibrational spectroscopy. Of specific interest is the solution of certain matrix equations to determine the type and frequency of the normal modes in polyatomic molecules. The application of perturbation techniques to a determination of some reliable force fields is also envisaged.

The matrix equations involved may be written in the form:

$$[GF - \Lambda]L = 0$$

where Λ are the eigenvalues and L the eigenvectors of GF, which is of dimension 3N-6 for a nonlinear N-atomic molecule. The solution for large molecules with low symmetry is impractical unless a computer is available. Perturbation involves an iterative process in which F is adjusted until the calculated and observed Λ agree.

(B) Rayleigh scattering of light

Principal investigator

Dr. Ellis R. Lippincott Professor Chemistry

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
201/66/013	1/66	In progress	0	0

Most of the theories dealing with the effect of the state and the solvent medium upon molecular spectra give rise to expressions for frequency and/or intensity shifts which contain, either implicitly or explicitly, the value of the mean polarizability, α, of the molecule under investigation. Frequently, this value is obtained from the measured refractive index or dielectric constant. Both of these measurements, however, may only approximate the true value of α, and cannot indicate anisotropy for the case where complete randomness of orientation is ruled out by the nature of the molecular environment.

The measurement of intensity of Rayleigh scattering of light, polarized parallel to and perpendicular to the direction of observation, gives both the mean polarizability α, and the anisotropy β:

$$I(\Psi) = K\left[\frac{2\beta^2}{15} + \frac{45\alpha^2+\beta^2}{45}\cos^2\Psi\right]$$

where $K = \frac{16\pi^4\nu^4}{c^4} NI_o$, fixed for a given system

$$\alpha = 1/3(\alpha_1+\alpha_2+\alpha_3)$$

$$\beta^2 = 1/2[(\alpha_1-\alpha_2)^2 + (\alpha_2-\alpha_3)^2 + (\alpha_3-\alpha_1)^2]$$

Ψ is the angle which the plane of polarization makes with the direction of observation.

This equation is derived with the assumption that all orientations of the molecule have equal probability, so that

cross products all have zero value. If this assumption is not true, and certain configurations are preferred due to molecular interaction, the measured variation of $I(\Psi)$ will deviate from that calculated. It is planned to write a program (probably using MAD) to calculate $I(\Psi)$ for many assigned values of α_1, α_2 and α_3, generating families of curves with which experimentally observed values may be compared.

This will be a simple, straightforward computation, performed for a large number (about 5,000) of sets of parameters. If significant and characteristic differences are found on comparison with data from actual systems, an effort will be made to find applicable correlation functions and test their usefulness in revising the equation for $I(\Psi)$.

(C) Calculation of solvent-solute interaction energy derivative terms

Principal investigator

Dr. Ellis R. Lippincott — Professor — Chemistry

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
201/66/012	1/66	In progress	0	0

Equations have been derived by Buckingham[1] through implementation of perturbation theory to describe frequency displacements of vibrational bands of polyatomic molecules upon condensation in a medium. The equations are given in the form

$$(1)\quad \omega_i - \omega_i^{(0)} = (8\pi^2 c^2 \omega_i)^{-1} \left\{ \langle U''_{ii} \rangle - 12(8\pi^2 c^2)^{-1} \left[\sum_j^{3N-6} \frac{\alpha_{iij}}{\omega_j^2} \langle U'_j \rangle \right] \right\}$$

for each normal vibrational frequency ω_i. The U_{ii} and U_i are derivatives of the solvent-solute interaction energy U expressed as a power series in Q_i, the normal coordinates of vibration, and averaged over all configurations; and the α_{iij} are the cubic anharmonic potential constants. It has been shown[2] that for linear triatomic and non-linear symmetrical triatomic molecules, utilization of isotopic species (HCN-DCN, for example) yields enough equations (1) to solve for the U_{ii} and U_i. This is accomplished by a transformation R=LQ to internal coordinates. This yields for the energy derivatives in HCN-DCN

$$(2)\quad \langle U'_j \rangle = \left(\frac{\partial U}{\partial Q_j}\right) = L_{1j}\left(\frac{\partial U}{\partial R_1}\right) + L_{3j}\left(\frac{\partial U}{\partial R_3}\right) \qquad j=1,3$$

$$\langle U''_{jj} \rangle = L_{1j}^2 \left(\frac{\partial^2 U}{\partial R_1^2}\right) + L_{1j} L_{3j} \left(\frac{\partial^2 U}{\partial R_1 \partial R_3}\right) + L_{3j}^2 \left(\frac{\partial^2 U}{\partial R_3^2}\right)$$

$$\langle U''_{22} \rangle = L_{22}^2 \left(\frac{\partial^2 U}{\partial R_2^2}\right)$$

Upon substitution of (2) into (1), six equations are obtained

which may be solved simultaneously for the six unknown derivatives. A computer program has been written to solve for these energy derivatives making use of matrix operations.

It has been found that this solution is quite sensitive to small changes in various input parameters. For example, the experimentally observed frequencies ω_i are known to at best $\pm$ 1 cm^{-1}. When a solution of the equations is accompanied by iteration of these frequencies over this range, a sizable variation in the resulting energy derivative terms is found. It is hoped that methods of reducing this sensitivity may be found. Further, there are a number of simple molecules to which this calculation may be applied - H_2S-D_2S, H_2O-D_2O, $C^{12}O_2$-$C^{13}O_2$, $C^{12}S_2$-$C^{13}S_2$, CH_3X-CD_3X, CH_4-CD_4, to name a few possibilities. When values for the various energy derivatives are found, then the contribution of the solvent effects to bond extensions and vibrational amplitudes may be found by equations derived by Mann[2]. These calculations will also be incorporated into the program which solves for the energy derivatives.

A fairly sizable number of calculations is anticipated. The sensitivity of the solution will require calculations in which some of the input parameters are varied, and adjustments in the program until the sensitivity is reduced. In addition, preliminary studies have indicated that in some cases the cross term $(\frac{\partial^2 U}{\partial R_1 \partial R_3})$ may be neglected, leaving an over-determined problem of six equations in five unknowns. In this case, six combinations for the five equations are found, and average values for the five remaining energy derivatives are found from the six solutions of these equations. This approach will be applied to some of the molecules listed above as experimental values are obtained.

References

[1] Buckingham, Trans. Faraday Soc. 56, 753 (1960)

[2] Mann, R. H., Ph.D. Thesis, Princeton University, 1965

(D) Studies of solute-solvent interactions

Principal investigator

Dr. Ellis R. Lippincott Professor Chemistry

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
201/66/011	1/66	In progress	0	0

In recently published papers conditions have been described under which the strong and specific interactions (e.g. of the type of H-bond-formation) can be separated from overall electrostatic interactions in solutions. The changes in the model used for the Onsager reaction field theory show that equations developed by Buckingham for the frequency shift in infrared absorption bands (and derived from the Onsager theory) are definitely valid; the solute entities expected to be the subject of the reaction field of the solvent medium (continuum) are the H-bonded solute-solvent complex molecules and not the free solute molecules.

Under conditions applied to these studies it was also found that polar solutes form weak stoichiometric complexes in solutions in nonpolar solvents. These complexes have been described as "collision complexes", and their formation seems to be an inherent property of the liquid state. It is assumed that in these cases the molecules of the nonpolar solvent enter the so-called primary solvation site forming the collision complex, and that the complex is further a subject of the reaction field of residual molecules present in the system. In ternary mixtures containing polar solute, polar and nonpolar solvents, the solute entities present are the complex solute-polar solvent (e.g. H-bonded complex) and the collision complex solute-nonpolar solvent. In ternary mixtures containing polar solute and two nonpolar solvents, two different collision complexes have been expected, and this has been experimentally verified.

The estimate of the interaction energy involved in the formation of collision complexes is of high interest. It seems to be possible to derive information about this energy from thermodynamic calculations of H-bond formation in gas phase

and in solution. This is based on the consideration that in gas phase the non-associated entities present are "free", whereas in solutions collision complexes are formed.

Two approaches to this problem of solute-solvent interactions will be investigated:

(1) Infrared frequency shifts

The solvent-caused frequency shifts in absorption bands of fundamental vibrations of a solute can be expressed as functions of the dielectric constant ϵ and the refractive index n of the solvent or solvent mixture. The experimental values of frequencies, dielectric constants and refractive indices can be correlated by means of the Buckingham equation written in the form

$$\Delta\nu/\nu^{\circ} = C_{00} + C_{10}\,(f\epsilon) + C_{01}\,(fn^2) + C_{20}\,(f\epsilon)^2 + C_{11}\,(f\epsilon \cdot fn^2) + C_{02}\,(fn^2)^2 + \ldots.$$

These calculations are in the regular matrix type least squares form.

(2) Calculation of unperturbed components of superimposed bands

Calculations of this type will be used for the study of vibrational absorption bands of complexes formed in solution. In many cases different complexes are present in the solution simultaneously. The occurrence of two or more close or superposed absorption bands results. The mathematical resolution of these complicated band systems is necessary in order to study the properties (frequencies, halfwidths, intensities) of unperturbed components of these systems.

The band shapes are expressed as Gauss, Lorentz, or mixed functions. The experimental band-complex curve is compared with the curve calculated from estimates of the number of bands present and their properties. Regular matrix type least square calculations are used in this work.

(3) Calculation of thermodynamic constants of H-bond formation in gas phase and in solution

The calculations will involve solution of the Scott equation as described under Project 201/66/010 below.

(E) Thermodynamic constants for charge transfer complex formation reactions

Principal investigator

Dr. Ellis R. Lippincott Professor Chemistry

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
201/66/010	1/66	In progress	0	0

The investigation of charge transfer complexes formed by various halogen acceptors and donor molecules containing group IV-V and group IV-VI bands is now under way as part of a general study of the structure and bonding of these molecules. The far infrared spectra will be examined for those complexes which can be obtained as solids. For those which are fairly stable in solution, but which cannot be obtained as solids, the Raman spectra will be obtained. These stable complexes, as well as more "normal" complexes of low stability, will also be investigated by the conventional ultraviolet and visible spectroscopic techniques to obtain equilibrium constants for the charge transfer complex formation reaction. From the temperature dependence of these equilibrium constants the enthalpies of complex formation will be calculated. The free energy and entropy for each formation reaction will also be calculated. The enthalpy of the formation reaction gives a measure of the relative strengths of the donor-acceptor bond in the complexes. This information will be correlated with the force constant of this coordinate bond obtained from infrared and Raman spectroscopic data.

There are several two-dimensional spectrophotometric equations that can be solved by non-iterative procedures. This work will concern the solution of the Scott equation:

$$\frac{[B]}{\frac{OAM}{[A]} - a_A} = \frac{1}{K(a_C - a_A)} + \frac{[B]}{a_C - a_A}$$

which describes the reaction $A + B \overset{K}{\rightleftarrows} C$, with $[B]\rangle\rangle\rangle[A]$ or $[C]$ and the absorbance by [B] subtracted mechanically. In this equation, OAM and K are the measured absorbance and equilibrium constant, respectively; a_A and a_C designate the molar absorbancy index of A and C, respectively; [A] and [C] are the concentrations of A and C in moles/liter; and [B] is the concentration of B in moles/liter or in mole fraction units. K and a_C are unknown. The input consists of the measured absorbances at each of several temperatures for pairs of solutions having the same [A] but different [B]. The temperature dependence of the K obtained from the Scott equation (the average of K's calculated for each pair of solutions) is then used to obtain the enthalpy by a least squares treatment of the following equation:

$$\ln K = -\Delta H/RT + C$$

The probable error in ΔH will be calculated by the method of Birge[1]. From the slope and intercept which were calculated in the least squares treatment, the equilibrium constant for the association reaction at 0° and 25°C can be calculated, and form this the free energy obtained through

$$\Delta F = - RT \ln K$$

and the entropy by

$$\Delta S = \frac{\Delta H - \Delta F}{T}$$

Reference

[1] Phys. Rev. 40, No. 2, 207 (1932).

(F) Spectroscopic laboratory measurements and their relation to upper atmosphere observations

Principal investigator

Dr. Joseph T. Vanderslice Professor Institute for Molecular Physics

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
202/66/008	2/66	In progress	0	0

Spectroscopic studies on the aurora and related phenomena must obviously be supplemented by both laboratory measurements and theoretical calculations in order to define the physical processes that occur in the upper atmosphere. High resolution spectrographic plate measurements, together with lower resolution intensity work, are being carried out with the view of determining Franck-Condon factors and electronic transition moments for those electronic transitions which are of importance in interpreting upper atmospheric phenomena.

The high resolution data are used to compute accurate potential curves from which one obtains the Franck-Condon factors. These, along with intensity measurements, serve to determine the electronic transition moments. With the resulting data, one is able to interpret the auroral measurements in terms of the physical processes that may be occurring.

References

Benesch, W., J. T. Vanderslice, S. G. Tilford, and P. G. Wilkinson, Potential Curves for the Observed States of N_2 Below 11 e.v., Astrophys. J., 1965

Benesch, W., J. T. Vanderslice, S. G. Tilford, and P. G. Wilkinson, Franck-Condon Factors for Observed Transitions in N_2 Above 6 e.v., Astrophys. J., 1966a

Benesch, W., J. T. Vanderslice, S. G. Tilford, and P. G. Wilkinson, Franck-Condon Factors for Permitted Transitions in N_2, Astrophys. J., 1966b

(G) A study of the Brackett alpha emission of galactic nebulae

Principal investigator

Dr. William Benesch	Associate Professor	Institute for Molecular Physics
	Research Consultant	Computer Science Center

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
202/66/007	2/66	In progress	0	0

One of the major tasks of radio astronomy has been the mapping of galactic hydrogen and the measurement of its motion. It is the purpose of the present investigation to provide a means of extending our knowledge of the galactic center and similar regions, the so-called HII regions, where the occurrence of ionized hydrogen and interstellar dust characterizes the bright emission nebular structure. These regions must emit, among other radiation, the 4.05 micron photons of the Brackett Alpha line arising from the $5 \rightarrow 4$ transition in atomic hydrogen. Experimental work is now under way to obtain measurements of such radiation.

In support of the experimental observations required in this program, it is important to have accurate calculations of such quantities as the infrared transmission of optical systems, the energy emitted from a source under specified conditions as a function of wavelength, the angle dependence of sensitivity of a dectector package, etc. Some of these problems have been undertaken by computer and others will be attacked presently. It is anticipated that as this project matures, the data collection will be made computer-compatible to facilitate its reduction.

(H) Determination of infrared line intensities, widths, and shapes

Principal investigator

Dr. William Benesch	Associate Professor	Institute for Molecular Physics
	Research Consultant	Computer Science Center

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
202/66/006	2/66	In progress	0	0

A vacuum infrared study of the properties of simple molecules is centered around a spectrometer whose output is digitized. Wavelength and intensity data are punched out as five digit integers to serve as input data to computer programs designed to compute line intensities, widths, positions, and shifts.

An investigation is under way to examine the problem of determining the degree of accuracy required in the spectroscopic data to yield a given degree of accuracy in computed line intensities and widths under various conditions. Central to such an investigation is a consideration of the interplay between random noise and instrumental smearing.

Initial computations in this area have indicated a range of values of line parameters which should be most sensitive to the input data. A further selection must now be made within this group of line parameters to reconcile the mathematical requirements with practical spectroscopic considerations.

(I) Intermolecular forces: the equation of state of dilute gases

Principal investigator

Dr. Andrew De Rocco	Assistant Professor	Institute for Molecular Physics

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
202/65/003	8/65	In progress	0	0

The statistical mechanics of dilute gases yields an expression for the thermal equation of state as a power series in the density. The coefficients of this series are known as the virial coefficients. There are two problems associated with these coefficients: the first is a strenuous exercise in combinatorial topology which, fortunately, has been worked out;[1] the second is an insidious integral problem that has eluded analytical computation for all but the lowest virial coefficients obeying drastically simplified force laws[2].

In earlier work on phases of this problem (carried out at Maryland, Colorado and Michigan) machine procedures were developed to compute with abundant precision the value of these coefficients for more realistic force laws. It is now proposed to compute additional coefficients for polyatomic molecules and for mixtures of simpler gases. The computation of third virial coefficients is an especially interesting problem because there have appeared in recent months theoretical estimates of the correction necessary to this coefficient for the presence of three-body forces[3].

In preparation for this long-range project two programs have been developed, essentially truncated integration by Simpson's rule, which have already been tested and used. These programs were developed on Projects Nos. 202/63/011 and 202/64/001. From the first of these there has appeared a publication jointly with M. J. Feinberg[4]. From the latter, in collaboration with Sherwood, there will appear a paper on gases of globular molecules[5].

It is planned to perform a definitive comparative study of the first three virial coefficients for all "realistic" potential models and a complete survey and review of the equilibrium properties of gaseous mixtures.

References

[1] G. E. Uhlenbeck and G. W. Ford, Studies in Statistical Mechanics Vol. I (North-Holland, Amsterdam, 1962).

[2] W. G. Hoover and A. G. De Rocco, J. Chem. Phys. 34, 1059 (1961); A. G. De Rocco and W. G. Hoover, J. Chem. Phys. 36, 916 (1962); W. G. Hoover and A. G. De Rocco, J. Chem. Phys. 36, 3141 (1962); A. G. De Rocco and W. G. Hoover, Physica 28, 839 (1962).

[3] R. D. Present and H. W. Graben, Abstract EF4 of the September 1965 Meeting of the American Physical Society; A. E. Sherwood, A. G. De Rocco and E. A. Mason, to be published.

[4] M. J. Feinberg and A. G. De Rocco, J. Chem. Phys. 41, 3439 (1964); R. H. Fowler, H. W. Braben, M. J. Feinberg and A. G. De Rocco, J. Chem. Phys. (in press).

[5] A. E. Sherwood and A. G. De Rocco, to be published.

(J) The evaluation of Franck-Condon factors for diatomic molecules

Principal investigator

Dr. Ellis R. Lippincott — Professor — Chemistry

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
201/65/007	6/65	In progress	0/8	0/8

(K) Shock tube measurement on relaxation time of hydrogen

Candidate: B. Ouyang — Department: Physics and Astronomy
Degree: Ph.D.

Principal advisor: Dr. J. M. Burgers

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
205/65/046	6/65	In progress	0/33	0/33

(L) Microwave spectroscopy studies

Principal investigator

Dr. L. C. Krisher — Assistant Professor — Institute for Molecular Physics

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
202/64/002	2/65	In progress	4/20	5/43

(M) Computation of vibration-rotation matrix elements for diatomic molecules

Principal investigator

Dr. William Benesch	Associate Professor	Institute for Molecular Physics
	Research Consultant	Computer Science Center

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
202/63/002	6/63	In progress	20/39	39/36

Although the dipole moment function is a most fundamental property of a molecule, particularly as regards its interaction with radiation, surprisingly little is actually known concerning this subject in spite of considerable theoretical speculation. Investigations will be conducted on the factors on which depend the infrared line intensities of molecular vibration-rotation bands. The current experimental effort is directed most actively toward the hydrogen halides, which exhibit unusual intensity variations in vibration-rotation lines in both the fundamental and overtone bands. From the data on line intensities one may compute dipole transition matrix elements which, properly interpreted through accurate rotationally perturbed vibrational wave functions, will yield a dipole moment function for the molecular ground state.

Very similar techniques may be applied to the computation of relative intensities in the visible and ultraviolet. Thus, a study of ionizing transitions in CO is currently under way in an extension of the method used for the infrared.

In the study of the properties of simple molecules, particular stress has been placed on nitrogen as a result of the availability of high precision data from the vacuum ultraviolet region. Extensive calculations of potential curves, Franck-Condon factors, and r-centroids for a number of states and bands in nitrogen have led to a better understanding of several molecular mechanisms including the processes responsible for auroral emission bands. Accordingly, it should now be possible by a rather simple spectroscopic measurement to determine electron

temperatures in the auroral zone. A party from the Institute for Molecular Physics visited Ft. Churchill, Manitoba in February to study the aurora from this point of view.

References

[1] Influence of the vibration-rotation interaction on the infrared line intensities of diatomic molecules, W. Benesch, Jour. of Molecular Spectroscopy, Vol. 15, No. 2, Feb. (1965) 140.

[2] Potential curves of nitrogen below 12 ev., W. Benesch, J. T. Vanderslice, S. G. Tilford and P. G. Wilkinson, Astrophys. J. 142, 1227 (1965) October.

[3] Franck Condon factors for observed transitions in N_2 below 6 ev., W. Benesch, J. T. Vanderslice, S. G. Tilford and P. G. Wilkinson, Astrophys. J. 143, 000 (1966) January.

[4] Franck Condon factors for permitted transitions in N_2. W. Benesch, J. T. Vanderslice, S. G. Tilford and P. G. Wilkinson, Astrophys. J. 144, 000 (1966) July.

[5] Excitation rates in the auroral nitrogen second positive group. W. Benesch, J. T. Vanderslice and S. G. Tilford, J. Atm. Terr. Phys. (in press).

[6] A summary of observed absorption lines of room temperature molecular nitrogen between 1060 and 1520 angstroms, V. B. Franklin, R. H. Naber, S. G. Tilford, P. G. Wilkinson, W. Benesch and J. T. Vanderslice, Astrophys. J. Suppl. 115 (1966).

[7] Higher approximations in the Rydberg-Klein-Rees method. J. T. Vanderslice, R. Davies and S. Weissman, J. Chem. Phys. 43, 1075 (1965).

[8] Validity of the Jarmain-Sandeman series for calculating potential curves of diatomic molecules, R. H. Davies and J. T. Vanderslice, Can. J. Phys. (in press).

[9] Second order WKB corrections to Rydberg-Klein-Rees potential curves, R. H. Davies and J. T. Vanderslice, J. Chem. Phys. (in press).

(N) Rydberg-Klein-Rees procedure for determination of alkali metal potential energy curves

Principal investigator

Dr. Joseph T. Vanderslice	Professor	Institute for Molecular Physics

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
202/63/008	1/64	In progress	2/11	6/27

(O) Self-consistent field calculations

Principal investigator

Dr. Joseph T. Vanderslice	Professor	Institute for Molecular Physics

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
202/63/006	11/63	In progress	0/24	27/21

(P) Vibrational calculations

Principal investigator

Dr. Ellis R. Lippincott	Professor	Chemistry

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
201/64/004	10/64	10/65	0	0/9

2. Nuclear physics and engineering

The twenty-five projects described in this section are being conducted by the Nuclear Physics Group of the Department of Physics and Astronomy and by the Nuclear Engineering group in the Department of Chemical Engineering. Information on two additional projects, completed during the first half of 1965, was presented in the Semiannual Status Report.

New projects

302/65/021	Dynamic study of H-Zr system for nuclear reactor control
302/65/020	Relative reactivity worths of neutron absorbing materials for various geometries
302/65/019	Effective reactivity control by combinations of neutron absorbers in nuclear reactors
302/65/018	Determination of internal flux distributions in lumped highly absorbing materials using the nuclear reactor
302/65/017	Nuclear reactor reactivity measurements from neutron generation statistics
205/65/054	Nuclear reaction analysis

Continuing projects

205/65/050	Study of the B^{10} $(He^3, \alpha)Be^8$ and $B^{10}(He^3,\alpha)B^{9*}$ reactions
205/65/047	Elastic scattering of protons by Beryllium 9
302/65/013	Nuclear spectroscopy using nuclear reactor neutrons
205/65/042	Study of the reaction $N^{14}(He^3,\alpha)N^{13*}(p+C^{12})$
205/65/040	Analysis of $C^{14}(p,p)C^{14}$ and $N^{14}(p,p)N^{14}$
302/65/008	Design of a graphite subcritical nuclear reactor
205/64/026	Nuclear reaction theory
205/64/021	Nuclear structure physics research

205/64/013	Velocity gauge calculation
205/64/008	Calculation of particle energy as a function of Hall voltage
302/63/004	Nuclear reactor calculations
205/63/015	Multi-particle breakup
205/63/014	Magnet calibration
205/63/013	Reaction kinematics

Completed projects

205/65/043	R-matrix calculation of cross sections
302/65/010	Some effects of temperature on the criticality of the University of Maryland reactor
205/65/033	Nuclear reaction $Be^{9}(p,p)Be^{9}$
205/65/030	Gamma ray spectra analysis
205/63/004	Elastic scattering of protons by C^{13} nucleus

(A) Dynamic study of H-Zr system for nuclear reactor control

Candidate: Ralph Lightner
Degree: Ph.D.
Department: Chemical Engineering

Principal advisor: Dr. Dick Duffey

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/021	10/65	In progress	0	0

The reactivity of a nuclear reactor can depend on the neutron moderating properties of the system. Varying the hydrogen content is a possible way to alter the moderation. Experimental work is underway to study the changes of hydrogen content of nuclear reactor materials and the associated reactivity variations.

Computer calculations are necessary to reduce experimental data taken in connection with this project and to perform a parametric evaluation of certain transport characteristics. The data consist of a large number of experimental points. Calibration curves are to be read and other computations performed. For example, the gas flow rates will be integrated over the period of the runs to obtain a total mass transfer. In addition, criticality and kinetic behavior of the reactor system may be calculated.

FORTRAN codes are being written to perform these tasks. Nuclear reactor codes already in use will be applied.

(B) Relative reactivity worths of neutron absorbing materials for various geometries

Candidate: Malcolm Ross
Degree: M. S.
Department: Chemical Engineering

Principal advisor: Dr. Dick Duffey

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
302/65/020	10/65	In progress	0	0

The project consists of the measurement and subsequent analysis of the relative reactivity worths of a wide range of neutron absorbing materials. Since the reactivity worth of a specified amount of neutron absorber is strongly dependent on how it is arrayed, the neutron absorber properties of each of these materials will be investigated over a wide range of geometrical configurations. The significance of this type of study in nuclear reactor design is to obtain an optimization in the amount and configuration of any type of control material to yield a maximum reactivity effect.

Due to the complexity of the analysis, computer codes are to be utilized to determine the ability of various calculational models to reproduce experimental results. These models will then have been tested over a wide range of neutron absorber materials and hence a method will be determined which will accurately predict reactivity effects of these materials.

References

[1] Fisher, J. R., The utilization and effectiveness of linear arrays of neutron absorber filled tubes as control rods in water moderated reactors, Ph. D. Dissertation, University of Maryland.

[2] Pomraning, G. C., Control Worth of B_4C Rods, GEAP-3800.

(C) Effective reactivity control by combinations of neutron absorbers in nuclear reactors

Candidate: Laurence Kopp
Degree: Ph.D.
Department: Chemical Engineering
Principal advisor: Dr. Dick Duffey

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/019	10/65	In progress	0	0

A primary factor in the safety of nuclear reactor operation is limiting the amount of reactivity worth of any one individual control rod so that an accident involving the loss of a rod from the core will not result in significant reactivity addition. Rod worth can be greatly influenced by the operating pattern of adjacent rods. The reactivity worth of a given rod may increase by a factor of two or more depending on the spectrum perturbations caused by adjacent rods. One approach to the safety problem is to utilize mixtures of resonance and thermal neutron absorbers for control rods so that neutron spectral shifts will not cause significant changes in the absorption rates of the rods.

Available neutron absorbers, including many of the rare earths, will be combined, and reactivity measurements of their worth as a function of neutron spectrum changes will be made. Analytical methods will also be used to determine the validity of such for predicting control rod worth. The computer codes to be used will consist of the normal group constant generators such as MUFT, TEMPEST, etc., and one- and two-dimensional flux and reactivity codes such as AIM and PDQ.

(D) Determination of internal flux distributions in lumped highly absorbing materials using the nuclear reactor

Candidate: Richard Kern
Degree: Ph.D.
Department: Chemical Engineering

Principal advisor: Dr. Dick Duffey

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/018	10/65	In progress	0	0

The determination of the internal neutron flux distributions in lumped highly absorbing materials is extremely important in the design of burnable poisons for control in large nuclear power reactors and in the design of control rods. This is a result of the fact that the worth of a nuclear poison material is dependent on the neutron absorption rate, and this latter quantity is dependent on the neutron flux distribution inside the material. Also, the rate at which the nuclear poison depletes is dependent on the internal neutron flux distribution. Little work has been done on this important problem to date.

The project plans include the experimental determination of the internal neutron flux distribution in lumped highly absorbing materials using the nuclear reactor. Also, the depletion effects as a function of irradiation will be investigated.

The experiments will cover the use of a wide variety of materials in many different geometries, such as B_4C cylinders. The ability to calculate these internal neutron flux distributions is of prime importance. Computer codes will be used extensively for comparison with the experimental results. These computational methods will employ the exact theory for the calculation of neutron flux distributions.

The main references for this work are the reports published by Allis-Chalmers covering the limited work performed with Gadolinium Oxide cylinders. Among the codes to be used will be the SOFOCATE and DECYGAD codes.

(E) Nuclear reactor reactivity measurements from neutron generation statistics

Candidate: Agustin Diaz
Degree: Ph.D.
Department: Chemical Engineering

Principal advisor: Dr. Dick Duffey

			Computer time	
			Reporting	
Project No.	Initiated	Completed	period	Total
302/65/017	9/65	In progress	2/19	2/19

The purpose of this project is the correlation of neutron population statistics to the absolute measurement of reactivity in subcritical configurations of the University of Maryland nuclear reactor.

The computational work to be performed under this project involves the reduction of the statistical data obtained from measurements of the changes in the neutron level for static core conditions. It will also involve the independent calculation of the reactivity for different fuel assemblies by conventional computational methods.

Some of the computer codes that will be used are:

GAM-1. This code is prepared for the calculation of the slowing down spectrum in either the P.1 or B.1 approximation using 68 energy groups of neutrons with a constant lethergy width of .25.

TEMPEST II. This code is a neutron thermalization code based upon the Wigner-Wilkins approximation for light moderators. The code provides microscopic and macroscopic cross-section averaged over the thermal neutron spectrum.

PDQ. This is a two dimensional multigroup, multi-region diffusion code. It calculates the eigenvalue solution of the diffusion equations, using as inputs the outputs from GAM-1 and TEMPEST II.

(F) Nuclear reaction analysis

Principal investigator

Mr. David Nelson	Graduate Student	Physics and Astronomy

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
205/65/054	8/65	In progress	0/20	0/20

The analysis of nuclear reactions can often be simplified by the use of a well written, easy to use computer program. The investigator has written programs in FORTRAN II and MAD which have stressed input and output simplicity so that the user can determine the results with a minimum of effort. For example, "Comp 1" is a FORTRAN II program which will theoretically calculate and plot the energy as a function of angle for any nuclear reaction using only two data cards. This program has been used extensively and is filed in several libraries for future use. More recent work has used FORTRAN IV and has incorporated Calcomp plotting routines.

It is planned to write a program which will analyze data taken from a 512 channel analyzer. Its purpose will be to perform calculations on spectra taken from the analyzer and reduce the data to a form which is more easily interpreted by the experimenter. This program will also be made available to libraries for future use.

(G) Study of the $B^{10}(He^3, p\alpha)Be^8$ and $B^{10}(He^3, \alpha)B^{9*}$ reactions

Candidate: C. S. Han — Physics and Astronomy
Degree: M. S.
Principal advisor: Dr. H. D. Holmgren

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/050	7/65	In progress	7/17	7/17

(H) Elastic scattering of protons by Beryllium 9

Candidate: B. T. Mo — Physics and Engineering
Degree: Ph.D.
Principal advisor: Dr. W. F. Hornyak

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/047	6/65	In progress	16/10	16/0

(I) Nuclear spectroscopy using nuclear reactor neutrons

Candidate: K. K. Mehta — Chemical Engineering
Degree: Ph.D.
Principal advisor: Dr. Dick Duffey

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/013	6/65	In progress	2/45	2/45

(J) Study of the reaction $N^{14}(He^{3}, \alpha)N^{13*}(p+C^{12})$

Candidate: T. S. Bhatia — Physics and Astronomy
Degree: Ph.D.

Principal advisor: Dr. J. C. Armstrong

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/042	4/65	In progress	3/30	3/30

(K) Analysis of $C^{14}(p,p)C^{14}$ and $N^{14}(p,p)N^{14}$

Candidate: W. R. Harris — Physics and Astronomy
Degree: Ph.D.

Principal advisor: Dr. J. C. Armstrong

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/040	3/65	In progress	10/16	10/16

(L) Design of a graphite subcritical nuclear reactor

Principal investigator

Dr. F. J. Munno — Assistant Professor — Chemical Engineering

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/008	2/65	In progress	5/35	5/35

(M) Nuclear reaction theory

Principal investigator

Dr. William MacDonald	Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time Reporting period	Total
205/64/026	11/64	In progress	4/27	9/10

Work will continue on the application of the Shell Model Approach to Reaction Theory (SMART) [1] to the analysis of nuclear reactions in which both resonant and non-resonant processes contribute. This project has two principal goals. The first is to demonstrate the feasibility of a completely consistent calculation of reaction amplitudes using shell model wave functions as intermediate state functions in the resonant amplitude. The second goal is to develop machine codes for such calculations which have sufficient speed and flexibility to permit detailed studies of the relation between the finite model potential and the effective interaction used in shell model calculations.

In the portion of the project already completed, the theory has been used to describe single particle resonances near zero energy and to demonstrate that configuration mixing in the continuum can be treated by the use of a binding potential [2]. The numerical computations were essential in evaluating the corrections to a perturbation treatment of the residual one-body interaction by comparison with the exact resonance amplitude.

These results have now been used as the basis for a further calculation of the widths and level shifts for all the $J = 1^-$, $T = 1$ levels in O^{16} arising from particle-hole configurations [3]. These calculations were based on certain dispersion relations discovered during the work on one body resonances during the past year. The results obtained for widths were in reasonable agreement with available experimental data. The values obtained for the level shifts were comparable to the level shifts, as suspected would be the case. However, these shifts were found to be nearly independent of the incident

particle energy and therefore could be described by an energy independent effective interaction.

These computations employed a square well for the shell model potential and were therefore subject to criticism, since this potential does not reproduce the low energy scattering. This is now being remedied by the development of a computer program which will use the more realistic Saxon-Woods potential for the calculation of both scattering and bound state wave functions. The program, known as ABACUS, has already been used to repeat the analysis of the resonant $d_{3/2}$ neutron and proton scattering on O^{17} and F^{17} respectively and to determine a spin-orbit potential which fits both these resonances and the $d_{5/2}$ bound states in these nuclei.

The remainder of the program requires the integration of subroutines for the evaluation of shell model matrix elements, the diagonalization of energy matrices, and the calculation of interaction matrix elements between two-particle bound and continuum states. Some of these routines have been obtained but require further modification and checking out.

With the development of the ABACUS program a number of studies are planned on the reaction amplitudes for photonuclear, resonant scattering, and charge exchange reactions. The significance of these studies for the program of unified nuclear reaction theory has been discussed in past reports. Support of the theoretical work continues to be provided by NASA under research grant NsG 642. However, this grant does not include funds for computations. The support for computations provided by NsG 398 is therefore vital to the useful application of the theoretical results.

References

[1] MacDonald, W. M., Nucl. Phys. 54, 393 (1963); 56, 636 (1964); 56, 647 (1964)

[2] Garside, L. and W. M. MacDonald, Phys. Rev. 138, B582 (1965)

[3] Garside, L., doctoral dissertation, University of Maryland

[4] Garside, L. and W. M. MacDonald, International Conference on the Study of the Nuclear Structure by Neutrons (Antwerp) (1965)

(N) Nuclear structure physics research

Principal investigator

Dr. Nathan S. Wall	Associate Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/64/021	10/64	In progress	16/44	16/44

There are a number of problems in nuclear structure physics which are currently being analyzed through the use of nuclear models. These models essentially enable one to formulate the particular problem under investigation in terms of series of differential equations derived from the Schrödinger equation. Various numerical techniques are used for the solution of these equations. A number of programs have been developed at other laboratories, and in the past year have been put into operation here, and several programs, including one for Fourier transforming single particle wave functions, have been written here.

The particular programs in use here are:

(1) Nuclear kinematics

(2) Distorted wave Born approximation (ORNL program JULIE)

(3) Single particle Schrödinger equation (BNL - ABACUS II)

(4) Quasi-elastic scattering from single particle states.

During the next year these programs will all be in use and new ones will be added to handle elastic and inelastic electron scattering and a distorted wave version of quasi-elastic scattering.

(o) Velocity gauge calculation

Principal investigator

Dr. Jerry B. Marion	Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/64/013	6/64	In progress	0/25	5/56

(p) Calculation of particle energy as a function of Hall voltage

Principal investigator

Dr. James C. Armstrong	Assistant Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/64/008	3/64	In progress	1/2	8/1

Interim results on this project, relating to analysis of data for $C^{12}(p,p)C^{12}$, are described in University of Maryland Department of Physics and Astronomy Technical Report 488, August 1965. The computer program developed for this analysis will also be applied to the data from $C^{14}(p,p)C^{14}$ on Project 205/65/040.

(Q) Nuclear reactor calculations

Principal investigator

Dr. Dick Duffey	Professor	Chemical Engineering

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
302/63/004	2/64	In progress	35/56	90/33

Objectives:

Calculations relating to the core characteristics of the nuclear reactor are desired for both steady state and kinetic behavior. Studies will include the effect of insertion of foreign materials in the core, e.g. neutron absorbing materials of use in reactor control; void effects will also be studied. Correlation of computer predictions with actual measurements will be done. This will support both research work and projection courses, e.g. in Nuclear Reactor Engineering, which are expected to lead to theses.

Related calculations on the radiations produced by the nuclear reactor will be made, e.g., analysis of the gamma ray and beta ray emission of activated materials.

The following is information on some of the computer codes to be tried; these codes pertain mostly to reactor physics analysis and related studies concerning nuclear reactor operations. Much of this is based on the Argonne National Laboratory Computer Library work.

1) MUFT-5 - This program will solve the P1 or B1 multigroup neutron equation for the first two Legendre coefficients of the directional neutron flux - flux and current - and the isotropic and anisotropic components of the slowing down densities due to a cosine-shaped neutron source. Hydrogen may be treated exactly or in a Selengut-Goertzel approximation. For energy degradation by heavy elements, a Grueling-Goertzel approximation is available. Slowing down of neutrons

by inelastic scattering and removal of neutrons by capture and fission resonances are included. Only the non-thermal energy range is considered.

2) WANDA-5 - This is a numerical solution of the one-dimensional few-group neutron diffusion equations. One to eight energy groups may be used and rectangular, cylindrical, or spherical geometry formulations are available. The program will vary buckling or neutron poison cross section in any subset of regions, or the position of one or more interfaces separating regions, to find a specified critical eigenvalue. One-iteration or fixed source problems may be calculated and adjoint solutions may be obtained. All one-group problems are treated as one-iteration problems.

3) GAM-I - This program computes the slowing down spectrum in either the Pl or Bl approximation using 68 groups of neutrons with a constant group width DU-0.25. The code calculates multigroup constants for up to 32 fast groups.

4) TEMPEST-II - Tempest-II is a neutron thermalization code based upon the Wigmer-Wilkins approximation for light moderators and the Wilkins approximation for heavy moderators. A Maxwellian distribution may also be used. The model used may be selected as a function of energy. The second-order differential equations are integrated directly rather than transformed to the Riccati equation. The code provides microscopic and macroscopic cross-section averages over the thermal neutron spectrum.

5) PDQ - This is a dimensional multi-group, multi-region diffusion code. It calculates the eigenvalue solution of the diffusion equations, using as inputs the outputs from GAM-I and TEMPEST-II.

There will be a number of other codes used, including three dimensional codes, burn-out and reactivity codes, spectrum codes and disadvantage factor codes for nuclear reactors. Other codes related to nuclear reactor operations will also be used; for example, data from the gamma ray multichannel analyzer will be processed to identify kinds of and amounts of nuclides activated in neutron activation analysis work. There will also be codes bearing on neutron and gamma ray shielding,

heat transfer and stress analysis. Monte Carlo techniques may be applied to neutron and gamma ray problems. All of these codes will be compatible with the IBM 7094 and will be programmed in the FORTRAN language.

During the reporting period, this research resulted in a Ph.D. dissertation by Mr. J. R. Fisher: The utilization and effectiveness of linear arrays of neutron absorber filled tubes as control rods in water moderated nuclear reactors, June, 1965.

This work is now being continued and extended to investigate the properties of the rare earths samarium to lutecium with the goal of obtaining maximum reactivity control in a nuclear reactor with the use of a minimum amount of absorber material. This promises economies in materials as well as simpler designs.

(R) Multi-particle breakup

Candidate: C. Moazed
Degree: Ph.D.
Physics and Astronomy

Principal advisor: Dr. H. D. Holmgren

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
205/63/015	7/63	In progress	4/14	20/32

(S) Magnet calibration

Principal investigator

Dr. Jerry B. Marion — Professor — Physics and Astronomy

Project No.	Initiated	Reactivated	Computer time Reporting period	Computer time Total
205/63/014	6/63	2/65	0/1	1/12

(T) Reaction kinematics

Principal investigator

Dr. Jerry B. Marion — Professor — Physics and Astronomy

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
205/63/013	11/63	In progress	0/2	2/9

(U) R-matrix calculation of cross sections

Candidate: M. (Ball) Baggett — Physics and Astronomy
Degree: Ph.D.

Principal advisor: Dr. James C. Armstrong

Project No.	Initiated	Terminated	Computer time: Reporting period	Computer time: Total
205/65/043	5/65	10/65	0	0

This thesis project has been dropped.

(V) Some effects of temperature on the criticality of the University of Maryland reactor

Candidate: J. L. O'Brien — Chemical Engineering
Degree: M. S.

Principal advisor: Dr. Dick Duffey

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/010	3/65	9/65	0/8	0/8

This thesis has been successfully completed.

(W) Nuclear reaction $Be^9(p,p)Be^9$

Principal investigator

Dr. William Hornyak	Professor	Physics and Astronomy

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
205/65/033	2/65	9/65	3/38	3/46

Results:

A computer program was written to compute the kinematics of this reaction and then generalized to compute the kinematics of any nonrelativistic two body reaction. This program, called 'COMP I', has been made available to all members of the research group and is expected to be of considerable use in the future study of nuclear reactions.

(X) Gamma ray spectra analysis

Principal investigator

Dr. F. C. Young	Visiting Assistant Professor	Physics and Astronomy

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
205/65/030	1/65	9/65	0/15	0/16

Results:

This project has been terminated; the experimental data were not amenable to analysis by the proposed curve-fitting procedure.

(Y) Elastic scattering of protons by C^{13} nucleus

Candidate: V. Latorre — Physics and Astronomy
Degree: Ph.D.

Principal advisor: Dr. James C. Armstrong

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/63/004	4/63	9/65	4/52	15/32

Results:

This dissertation project has been successfully completed. The dissertation is entitled "Proton Elastic Scattering from C^{13}".

3. Physics and engineering of fluids

The seventeen projects in this section originate in the Departments of Aerospace Engineering and Chemical Engineering; the Institute for Fluid Dynamics and Applied Mathematics, and the Atmospheric and Space Physics Group of the Department of Physics and Astronomy. Four other projects, completed during the first half year, were described in the Semiannual Status Report.

New projects

302/65/016	Condensation of immiscible mixtures
302/65/015	Entry region mass transfer in an annulus

Continuing projects

301/65/008	Nonequilibrium blunt body flow
203/65/013	Unsteady flow over a flat plate in radiation gasdynamics
302/65/011	Kinetic study of absorption of 2.4-D in water by activated carbon in a fixed differential bed
303/65/015	A study of the relaxation of the Balescu-Lenard equations
301/65/007	Rotational flow over two-dimensional bodies using the method of integral relations
301/64/006	Non-steady state heat transfer in hypersonic flow
301/64/004	Compressible laminar boundary layer on elliptic cones by the method of integral relations
302/64/004	Momentum transfer of viscoelastic fluids in smooth-walled conduits
302/64/007	Dispersion coefficients in flow reactor vessels
301/64/003	Hypersonic flow about elliptic cones by the method of integral relations

302/64/005	Predicting rate of mass transfer in drop-wise liquid extraction
303/64/001	Numerical studies of boundary layer in-stability and turbulence
205/63/030	Langmuir and hot probe characteristics

Completed projects

301/64/005	Plane flow of a radiating gas
302/64/003	Diffusion mechanisms in ion exchange

(A) Condensation of immiscible mixtures

Candidate: Charles Henderson
Degree: Ph.D.
Chemical Engineering
Principal advisor: Dr. Joseph M. Marchello

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/016	7/65	In progress	0/50	0/50

Much work has been done in the area of condensation of pure vapors both with and without the presence of a noncondensible gas [1,2]. By assuming the pure vapor system to have certain properties, a theoretical expression was derived by Nusselt in 1916 which related several physically measurable quantities of the condensing system. The heat transfer coefficients of pure vapors condensing on a vertical surface, when calculated from this relationship, were within close agreement with those obtained from experiment. Other investigators have modified the equation to better fit their data, but the Nusselt form of the equation is generally preserved.

This investigation will attempt to bridge the gap between pure experimental investigations and the situations encountered in practice. In this study, the investigations will start at the simplest level, that of condensation of a pure vapor on a cold tube. The research will then be expanded in steps so as to eventually cover the final complex case. During all of these steps the data will be analyzed and compared with existing information for a check on equipment and experimental procedure. Most of the computer work will therefore involve fitting curves to physical properties and determining nonlinear coefficients for a working model of the experimental system.

References

[1] Colburn, A. P., and O. A. Hougen, Ind. Eng. Chem., 26, 1178 (1932)

[2] McAdams, "Heat Transmission", New York, McGraw-Hill Book Company (1956)

(B) Entry region mass transfer in an annulus

Candidate: James Cermak — Chemical Engineering
Degree: Ph.D.

Principal advisor: Dr. Robert B. Beckmann

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/015	7/65	In progress	0	0

This study will obtain mass transfer as a function of geometry in the entry region of an annulus. Chemical, nuclear and mechanical engineering employ processes which have entrance regions. Use of the above geometrical information should enable the designer to predict effects in the entrance region, yielding a better understanding and design.

The variables studied will be diameter, length, and flow rate using a closed water loop. The data will be correlated with integrated concentration and velocity distributions and/or empirically.

Computational methods will be employed in data reduction, least squares fit of the data, formulation of a correlation, and treatment of theoretical and empirical models.

A doctoral thesis titled, "Entry-Region Heat Transfer in an Annulus" by R. F. Farman was accepted in January, 1965 and is currently being prepared for publication.

Some references are as follows:

[1] R. G. Deissler, NACA-TN-3016 (1953)
[2] J. H. Wiegand and E. M. Baker, AIChE TRANS., Vol. 38, p. 569 (1942)
[3] R. G. Deissler, NACA-TN-2410 (1951)
[4] R. G. Deissler, NACA-TN-2138 (1950)

(C) Nonequilibrium blunt body flow

Candidate: L. L. Perini
Degree: M. S.

Aerospace Engineering

Principal advisor: Dr. Walter L. Melnik

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
301/65/008	7/65	In progress	2/39	2/39

(D) Unsteady flow over a flat plate in radiation gasdynamics

Candidate: A. Y. Sachs
Degree: M. S.

Mathematics

Principal advisor: Dr. S. I. Pai

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
203/65/013	6/65	In progress	1/12	1/12

(E) Kinetic study of absorption of 2,4-D in water by activated carbon in a fixed differential bed

Candidate: E. R. Magtoto
Degree: Ph.D.

Chemical Engineering

Principal advisor: Dr. Robert B. Beckmann

Project No.	Initiated	Completed	Computer time Reporting period	Computer time Total
302/65/011	3/65	In progress	3/13	3/13

(F) A study of the relaxation of the Balescu-Lenard equation

Candidate: L. N. Foster
Degree: Ph.D.
Principal advisor: Dr. D. A. Tidman

Institute for Fluid Dynamics and Applied Mathematics

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
303/65/015	5/65	In progress	19/7	19/7

Interim results:

This project is an extension of a study of the Balescu-Lenard equation which was started by A. Dolinsky. The equation is believed to depict the time development of a plasma from a given initial distribution. The equation is of interest because it is believed to take into consideration the collective effects in the action of the plasma which are so important in its development. An understanding of some of the fundamental properties will aid in an understanding of physical processes in the laboratory, in space exploration, and in the study of the outer layers of the sun.

The equation, being a non-linear integro-differential equation, does not admit the use of advanced linear techniques. The maintenance of the meaningful physical constants requires the use of point differentiation formulas. The integrations are carried out by the straightforward Simpson's rule method. The plotting of the information directly on a plotter has aided greatly in the analysis of the operation of the program and in the rapidity with which the project has been able to proceed.

(G) Rotational flow over two-dimensional bodies using the method of integral relations

Candidate: Robert S. Reilly — Aerospace Engineering
Degree: M. S.

Principal advisor: Dr. Walter L. Melnik

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
301/65/007	2/65	In progress	3/58	4/3

The theoretical aspect of the problem has been completed and programmed for the 7094 machine. The program has just been debugged and is now ready to be used to calculate the flow properties around two dimensional bodies in a non-uniform flow field.

The input to the program is the Mach number distribution in front of the body. Various Mach number distributions will be specified and the flow properties calculated from the program will be compared.

The program uses a SHARE library subroutine designated FNOL2 to solve three simultaneous non-linear differential equations for the shock wave shape and the velocity, pressure, density, and Mach number along the body surface.

(H) Non-steady state heat transfer in hypersonic flow

Candidate: S. Schreier — Aerospace Engineering
Degree: Ph.D.

Principal advisor: Dr. S. I. Pai

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
301/64/006	1/65	In progress	15/5	15/36

Temperature and velocity profiles are to be found across the boundary layer of a semi-infinite flat plate accelerating from rest, taking into account the variation of $\rho\mu$ across the boundary layer. The problem is solved by expressing both the velocity and the enthalpy in terms of doubly infinite series in x and t, in which the coefficients are functions of certain carefully selected non-dimensional variables. Substitution of these series into the governing equations results in a series of ordinary differential equations which may be solved by computer.

The ordinary differential equations are solved by turning the given jury problem into a marching problem. The boundary conditions at the wall are assumed and the equations are integrated forward. Under the program, the computer checks to see if the proper limiting value is being approached as the independent variable increases. If it is not, then the computer changes the initial conditions and integrates again, and so on, until the correct solution is found, when the computer automatically stops. It is obvious that without the computer, this method of solution would not be practical.

(I) Compressible laminar boundary layer on elliptic cones by the method of integral relations

Principal investigator

Dr. Walter L. Melnik — Associate Professor — Aerospace Engineering

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
301/64/004	12/64	In progress	6/53	8/30

The equations governing a non-similar boundary layer are reduced to a set of ordinary differential equations by the method of integral relations [1]. The resulting system of first order non-linear differential equations must be integrated numerically with initial values obtained from the solution of non-linear algebraic equations. Calculations must be carried out in double precision arithmetic to obtain initial values. Integration of the lowest order approximation shows a completely unexpected behavior, while the initial values rapidly converge to the exact solution.

The differential equations are ill-conditioned around the origin. The results to date indicate that the lowest order terms of a power series solution about the origin are not adequate for starting the integrations. It is proposed to examine the properties of the solution in the neighborhood of the origin in some detail (e.g., calculate the next term of the series solution). Hopefully the integrations can then be carried out in single precision arithmetic, preferably with a variable step size under error control.

Initial values are calculated from non-linear algebraic equations by a combination of the methods of steepest descent and Newton-Raphson. Initial values have been obtained for one- and two-strip approximations, but so far we have failed to obtain a solution for the next higher approximation. Numerical integrations should be quite straightforward once proper initial values are established.

References

[1] Dorodnitsyn, A. A., "On a method of numerical solution of some non-linear problems of aero-hydrodynamics", Proceedings, 9th International Congress on Applied Mechanics, Brussels, Vol. 1, 485, 1957.

(J) Momentum transfer of viscoelastic fluids in smooth-walled conduits

Candidate: S. D. Cramer — Chemical Engineering
Degree: Ph.D.

Principal advisor: Dr. Joseph M. Marchello

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/64/004	11/64	In progress	0/45	1/10

Viscoelastic fluids constitute a class of fluids distinguishable by the elastic deformation which accompanies plastic deformation. As a shear field develops within a fluid elastic energy is stored which is subsequently released when the shear field dissipates. Physically this storage of energy manifests itself in the appearance of normal stresses within the fluid. These stresses, moreover, can be of either of two types; they may be either of a compressive or tensile character. In fully developed, steady state simple shearing motion these normal stresses are functionally related to the local shear rate. This phenomenon is a commonly observed property of high molecular weight polymer solutions and molten polymers.

The steady state shear behavior of these fluids is not generally characterized by a constant viscosity coefficient as in the case of Newtonian fluids. Instead, the viscosity is a highly non-linear function of shear rate, or, as some investigators suggest, shear stress. Many rheological models have been proposed to describe the viscosity function. Among these, the most successful, because of its relative mathematical simplicity, is the "power law" or Ostwald-de Waele model. Many useful engineering correlations are based upon this model.

The primary limitation of the power law and other models is the somewhat limited range of shear rates (or stresses) over which they are applicable. Under many circumstances this presents no difficulty. But, however convenient they may be for the particular situation, they do not present an unambiguous basis for comparing, interpreting and correlating viscosity data, as the characterizing parameters are generally functions of shear rate (or stress).

Analysis of a theoretical and several semi-empirical rheological models has produced sets of constitutive equations posesssing the necessary tensor characteristics. These equations yield, upon suitable manipulation, expressions for the viscosity as a function of shear rate. Preliminary results suggest a common origin for the viscosity functions suitable over the entire range of shear rates. The models analyzed then appear as approximations to this generalized viscosity function.

The relative simplicity of the power law and other empirical models is sacrificed by the introduction of the generalized viscosity function. However, it is theoretically satisfying and appears to possess a broader utility for describing, interpreting, and comparing viscosity data. Experimental confirmation of such conclusions is necessary. Parameter evaluation will progress along lines of a least squares fit of the generalized viscosity function to the experimental data. Polymer concentration and perhaps temperature dependence of these parameters will be examined.

Root extraction and numerical integration techniques will be necessary for evaluation of velocity profiles and volumetric flow rates in smooth walled cylindrical conduits. A statistical comparison with experimental data will follow. A set of master curves for parameter evaluation may be one of the primary products of the numerical treatment.

(K) Dispersion coefficients in flow reactor vessels

Candidate: Chan M. Park
Degree: Ph.D.

Chemical Engineering

Principal advisor: Dr. A. Gomezplata

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/64/007	10/64	In progress	1/10	1/14

Interim results:

A least squares program for correlating the dispersion coefficient with other flow parameters, with application to packed beds as well to tubular reactors, has been coded and checked. In addition, a program to compute the moments on a purely statistical basis is being written. Use of the computer will be made to check the flow properties of our experimental bed with those discussed in the literature.

(L) Hypersonic flow about elliptic cones by the method of integral relations

Principal investigator

Dr. Walter L. Melnik — Associate Professor — Aerospace Engineering

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
301/64/003	8/64	In progress	6/31	9/7

Hypersonic flow of an ideal gas about elliptic cones is to be calculated using the method of integral relations [1,2]. Numerical results have been obtained with the lowest order approximation for only one case because the differential equations are highly unstable with respect to unspecified initial conditions.

The terms in the differential equations responsible for the unstable behavior must be identified. It is expected that convergence to the desired boundary conditions can be improved by corrections obtained from equations linearized with respect to some basic approximation of the full solution. It is proposed to investigate other methods of solution, e.g. transforming the governing equations to the stream function planes [3] and then seeking some form of linearization of the resulting equations.

The governing differential equations must be integrated numerically using a variable step size under automatic error control. The method of finding unspecified initial conditions is crucial to the calculation. The search for the desired solution is guided by a comparison of previous trials with the best previous approximation [2]. More rational interpolation schemes have been unsuccessful.

References

[1] See Project 301/64/004.

[2] Melnik, Walter L., "Supersonic and hypersonic flow of an ideal gas about elliptic cones by the method of integral relations", Ph.D. Thesis, University of Minnesota, 1964.

[3] Stocker, P. M. and F. E. Mauger, "Supersonic flow past cones of general cross-section", J. Fluid Mech. 13, 383, 1962.

(M) Predicting rate of mass transfer in drop-wise liquid extraction

Candidate: W. B. Ellis — Chemical Engineering
Degree: Ph.D.

Principal advisor: Dr. Robert B. Beckmann

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/64/005	8/64	In progress	7/11	7/13

(N) Numerical studies of boundary layer instability and turbulence

Principal investigator

Dr. A. J. Faller	Research Associate Professor	Institute for Fluid Dynamics and Applied Mathematics

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
303/64/001	1/64	In progress	34/34	61/55

(O) Langmuir and hot probe characteristics

Principal investigator

Dr. Richard T. Bettinger	Assistant Professor	Physics and Astronomy

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
205/63/030	11/63	In progress	13/24	18/48

(P) 1) Boundary layer flow with thermal radiation transfer at low Prandtl numbers
2) Magnetohydrodynamic duct flow

Candidate: C. K. Tsao — Aerospace Engineering
Degree: Ph.D.

Principal advisor: Dr. S. I. Pai

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
301/64/005	9/64	9/65	23/9	23/20

This project has been successfully completed. The thesis is entitled "Plane flow of a radiating gas".

(Q) Diffusion mechanisms in ion exchange

Candidate: J. P. Copeland — Chemical Engineering
Degree: Ph.D.

Principal advisor: Dr. Joseph M. Marchello

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
302/64/003	8/64	9/65	2/59	4/0

Computational work on this project has been completed; the dissertation is now in preparation.

4. Physics and astronomy

This section describes fourteen projects in Particle Physics, Dosimetry, Atmospheric and Space Physics, and Astronomy. It corresponds to Sections 3 and 5 of the Semiannual Status Report. Four additional projects, completed or transferred during the first half year, were described in that report.

New projects

205/66/074	An analysis of neutral hydrogen fine structure of the milky way in the Perseus region
205/65/064	Stellar random velocities in the solar neighborhood
205/65/061	An analysis program for cosmic ray air shower data
205/65/056	Orbits in a magnetic dipole field

Continuing projects

205/65/051	Brightness distributions of galactic supernovae
205/65/038	H II region line profile analysis
302/65/014	Electron energy deposition
205/64/025	Weak interaction form factors
205/64/024	Studies in final state interactions
205/64/023	K Meson decay schemes and problems of weak interactions

Completed projects

205/65/041	Pilot study of galactic structure
205/65/032	The brightness distribution of the sun at 11 meters
205/65/029	Peierls mechanism in the Lee model
205/63/023	Bootstrap calculations

(A) An analysis of neutral hydrogen fine structure of the milky way in the Perseus region

Candidate: James J. Rickard
Degree: Ph.D.
Physics and Astronomy
Principal advisor: Dr. Gart Westerhout

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/66/074	1/66	In progress	0	0

This project is a continuation of a Pilot Study of Galactic Structure as Determined by 21-cm Observations in the Perseus Region (Project No. 205/65/041) which was submitted as the investigator's Master of Science thesis in August 1965. The data used in this completed project were obtained with the 300 foot radio telescope at the National Radio Astronomy Observatory in Green Bank, West Virginia, used in conjunction with the 90-channel DTM receiver. The present project's data were obtained with the same telescope but with the 100 channel autocorrelation receiver of the NRAO. The new receiver is a vast improvement over the old, allowing observations of the same (or better) quality in 1/30th the time. As a result many more observations of the same region of sky were taken, which makes it possible to significantly reduce the noise in the observations.

It is planned to analyze the newer, more complete data in a manner similar to that of the previous project, producing contour maps which aid the analysis of HI fine structure in the Galaxy. Due to the large number of line profiles to be handled (10,000) the 7094 computer will be an invaluable tool for sorting and analyzing the magnetic tape records.

(B) Stellar random velocities in the solar neighborhood

Principal investigator

Dr. Uco Van Wijk	Associate Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/064	12/65	In progress	0/20	0/20

Since not enough time has elapsed for complete relaxation, the distribution of stellar random velocities near the Sun is to some extent dependent on the initial conditions. In 1956, the investigator published numerical results based on simple physical assumptions concerning the initial conditions. This model gave good agreement with the observations. Since that time more data and better models for the galactic gravitational field have become available, so that it is desirable to carry out more detailed calculations.

The present planned calculations are in the nature of a test, though they will lead to a published paper. When these are completed, it is planned to obtain independent financial support for a more extensive program. The calculations consist of the numerical evaluation of integrals of the type:

$$\int f(r)\, g^{-1/2}(r)\, dr$$

over the interval in r for which g(r) is positive.

(C) An analysis program for cosmic ray air shower data

Principal investigator

Dr. Martin La Pointe	Assistant Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/061	11/65	In progress	0	0

This project will deal with the reduction and analysis of cosmic ray air shower data obtained at an experimental station on Mt. Chacaltaya in Bolivia. The site is located near the city of La Paz at an altitude of 17,200 ft. above sea level. Such a great altitude is desirable for this work since the atmospheric cover is about half of what it would be at sea level. Extensive air showers result when high energy primary cosmic rays of galactic and extragalactic origin interact and multiply in the atmosphere to produce a cascade or "shower" of charged particles which are spread over many acres. Primary cosmic rays of this energy ($>10^{15}$eV) occur so infrequently that their detection is possible only because of this amplification in the atmosphere.

The Bolivian Air Shower Joint Experiment (BASJE) was initiated in late 1959 as a result of discussions between members of the Laboratory for Nuclear Science, MIT; the Institute for Nuclear Studies, University of Tokyo; the Laboratorio de Fisica Cosmica, La Paz; and the University of Michigan. The experiment was to have as its basic purpose the search for extensive air showers initiated by primary cosmic gamma rays. In addition, it was to provide new information concerning the primary energy spectrum and the properties of high energy interactions from a detailed study of showers at high altitudes. The following year BASJE received the support of the United States Air Force Office of Scientific Research and the Japanese Ministry of Education. During the fall of 1960 and spring of 1961, the equipment arrived in Bolivia and the installation was in operation at the laboratory on Mt. Chacaltaya at an altitude of 5,200 m. The first useful

data were recorded on January 18, 1962, on which date the first peculiar "low mu" air shower with extremely few penetrating particles was recorded. A preliminary report on this and related results was made at the Fifth Interamerican Seminar on Cosmic Rays, held in La Paz in July 1962.

With the recognition of a distinct class of low mu showers, the main problem of the BASJE became that of possible anisotropy in the arrival directions of the low mu showers. Such anisotropy would constitute almost certain proof that the primaries are gamma rays since ordinary cosmic rays are highly isotropic. To decide this question a substantial increase in the data was required. This has occupied a major fraction of the effort during the four years of operation of the BASJE.

To date there is some evidence for such an anisotropy. When the arrival directions are plotted according to galactic latitude, no anisotropy is evident. However, when they are plotted according to right ascension, a possible anisotropy has become apparent. The probability that this anisotropy arises from a statistical fluctuation is about 1%. The details of these results and of others concerning the primary energy spectrum and the character of the nuclear active core of the air showers were presented at the Ninth International Conference of Cosmic Rays in London in September 1965. The direction of the anisotropy corresponds to the direction of the Virgo cluster of galaxies. Further accumulation of data is required to confirm this result. Such confirmation would be a major astrophysical discovery.

The data from each of the 41 detectors are recorded on paper tape at the experimental site. The tapes are mailed to the United States where the data are transferred to magnetic tape prior to its analysis by a basic IBM 7094 FORTRAN II program. This program performs a least squares fit on the data in order to obtain a shower size, arrival direction, and core location which best fits the data. These results are written upon magnetic tape and on three printed copies, all of which are used for subsequent analysis at the collaborating universities. Each shower is processed by the basic program in about 2 seconds. The average rate of data collection in Bolivia is ~6,000 showers per month. Thus the average monthly 7094 computational requirement is about three hours/month.

(D) Orbits in a magnetic dipole field

Principal investigator

Dr. Alex Dragt	Assistant Professor	Physics and Astronomy

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
205/65/056	9/65	In progress	0/20	0/20

The study of the motion of a charged particle in a magnetic dipole field is basic to an understanding of the Van Allen radiation. The particular problem which it is planned to attack is the long-time behavior of the so-called "adiabatically invariant magnetic moment." The approximate constancy of this quantity is responsible for particle trapping in the Van Allen radiation. It is hoped to determine the energy at which nonconservation sets in as a function of various orbit parameters.

Besides its interest for the Van Allen radiation, the behavior of the magnetic moment of a particle in a magnetic field is also of importance in the design of mirror machines aimed at controlled fusion.

The method of computation is to integrate directly the equations of motion for the charged particle trajectory, and then examine the time behavior of the magnetic moment. A tried and tested integration scheme is already available for this purpose.

The results of a preliminary calculation of this kind have already been described in the review article listed below.

Reference

Dragt, A. J., Trapped orbits in a magnetic dipole field, Reviews of Geophysics, 3, 255-298, 1965.

(E) Brightness distributions of galactic supernovae

Principal investigator

Dr. M. M. Komesaroff — Visiting Associate Professor — Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/051	7/65	In progress	0/18	0/18

(F) H II region line profile analysis

Candidate: K. W. Riegel — Physics and Astronomy
Degree: Ph.D.

Principal advisor: Dr. Gart Westerhout

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/038	3/65	In progress	4/19	4/19

Interim results:

During the summer of 1965 the observational part of the program was completed at the National Radio Astronomy Observatory. At the same time, most of the preliminary data reduction was accomplished at the observatory using its computational facilities. The analysis stage of the investigation is now well under way. The computational tasks remaining are contour plotting, channel-by-channel plotting, and some averaging of data to improve the signal-to-noise ratio.

(G) Electron energy deposition

Candidate: M. J. Kniedler
Degree: Ph.D.
Chemical Engineering

Principal advisor: Dr. Joseph Silverman

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
302/65/014	7/65	In progress	10/4	10/4

(H) Weak interaction form factors

Candidate: V. Yu
Degree: Ph.D.
Physics and Astronomy

Principal advisor: Dr. Sadao Oneda

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/64/025	9/64	In progress	4/54	4/57

Interim results:

The axial vector form factors of nucleons and hyperons are being considered. The N/D method is used to obtain the matrix elements which involve the strong interactions. The effects of the possible scalar resonances on the intermediate state integral are given special consideration. In addition, it is planned to study the problems related to the scalar resonances (e.g., η-meson decay) in order to obtain another check on the parameter used in previous calculations. The matrix elements are formulated by dispersion relations. The dispersion integrals were evaluated using subroutine GAL, obtained through the SHARE Library. GAL performs Gaussian or Lobatto numerical integration.

(I) Studies in final state interactions

Principal investigator

Dr. Claude Kacser	Assistant Professor	Physics and Astronomy

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
205/64/024	11/64	In progress	1/7	2/0

Interim results:

This project is specifically directed toward the study of rescattering effects in the three body problem. It is hoped to have some of the computational results ready for publication by the spring of 1966. Plans are to continue calculations relevant to predicting the magnitude of possible experimental effects in low energy nuclear physics. Computational techniques will involve straightforward evaluation of analytic functions (including logarithms of complex quantities). The computer provides the ability to rapidly search many possible reactions, and also to compute algebraic functions of complex quantities rapidly. It is not planned to attack the integral equation directly until this initial calculation is completed.

(J) K Meson decay schemes and problems of weak interaction

Principal investigator

Dr. Jogesh C. Pati	Assistant Professor	Physics and Astronomy

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
205/64/023	10/64	In progress	2/27	5/4

(K) Pilot study of galactic structure

Candidate: J. J. Rickard — Physics and Astronomy
Degree: M. S.

Principal advisor: Dr. Gart Westerhout

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/041	4/65	1/66	2/53	2/53

Results:

This project was successfully completed; the thesis is entitled "A pilot study of galactic structure as determined by 21-cm observations in the Perseus region".

(L) The brightness distribution of the sun at 11 meters

Candidate: W. M. Cronyn — Physics and Astronomy
Degree: M. S.

Principal advisor: Dr. W. E. Erickson

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/032	2/65	8/65	4/7	4/12

This project has been successfully completed. The thesis is entitled "Thermal emission of the sun at 26.3 MHZ". A presentation on "The Flux and Brightness Distribution of the Sun at 26 MC" was given at the 119th Meeting of the American Astronomical Society, August 3-6, 1965, at the University of Michigan. An abstract of this presentation appears in the Astronomical Journal, Vol. 70, November, 1965.

(M) Peierls mechanism in the Lee model

Principal investigator

Dr. Jogesh C. Pati	Assistant Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/65/029	1/65	1/66	0	0/24

This project has been completed and has resulted in a report entitled "V Θ Bound States and Uniqueness in the Three Partical Sector of the Lee Model", University of Maryland Department of Physics and Astronomy Technical Report No. 452, 1965.

(N) Bootstrap calculations

Principal investigator

Dr. Jogesh C. Pati	Assistant Professor	Physics and Astronomy

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
205/63/023	8/63	1/66	0	7/50

This project has been completed. A report resulting in part from it is "Dynamics and Symmetries of Nonleptonic Hyperon Decays; Scalar Meson Couplings" by D. Lǫebbaka and J. C. Pati, University of Maryland Department of Physics and Astronomy Technical Report No. 541, January, 1966.

5. Other computer-oriented research in the sciences

This section includes seven projects in the fields of biophysics, psychology, and medicine.

Continuing projects

206/65/041	Eye movement and psychophysical research
454/65/003	Clinical shock: A study of the biochemical response to injury in man
206/65/034	Variability of detection level in visual perception
303/65/013	Denaturation and renaturation of DNA molecule
206/64/024	Research investigations in human learning and statistical analysis of research data
206/64/003	Predictive mathematical models for performance on operant conditioning schedules

Completed project

206/65/043	Effect of violation of assumptions on the t-test of significance of intercorrelations

(A) Eye movement and psychophysical research

Principal investigator

Dr. R. M. Steinman — Assistant Professor — Psychology

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
206/65/041	5/65	In progress	0/19	0/19

(B) Clinical Shock: A study of the biochemical response to injury in man

Principal investigator

Dr. R. A. Cowley — Professor and Head — Thoracic Surgery

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
454/65/003	3/65	In progress	3/0	3/0

(C) Variability of detection level in visual perception

Candidate: S. M. Shaffer — Psychology
Degree: Ph.D.

Principal advisor: Dr. T. G. Andrews

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
206/65/034	2/65	In progress	0/36	0/37

(D) Denaturation and renaturation of DNA molecule

Principal investigator

Dr. N. S. Goel — Research Associate — Institute for Fluid Dynamics and Applied Mathematics

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
303/65/013	4/65	In progress	2/16	2/16

In order to explain the experimental data on de- and renaturation of the DNA molecule, three models of kinetics and equilibrium situation of the melting process and its inverse have been proposed: (1) Zipper Model; (2) Random Model; and (3) Modified Ising Model. In the first model it is assumed that the hydrogen bonds break sequentially (like the opening of a zipper); in the second, that the bonds break at random; and in the third, that the breaking of neighboring pairs of bonds is correlated. In the third model, the correlation between nearest neighbor bonds is similar to the correlation between pairs of electron spins in the Ising model of ferromagnetism. ('Spin up' in the latter model corresponds to 'intact bond' in the DNA model; 'spin down', to 'broken bond.')

The first model has been applied to the DNA molecule with one kind of hydrogen bond only. The zipping and unzipping is considered to be the result of a succession of chemical reactions. Both equilibrium and kinetic situations have been considered. Calculations have been made for the average fraction of bonds intact, its time variation and its dispersion about the mean.

The second and third models have been applied also to the DNA molecule with both kinds (A-T and G-C) of hydrogen bonds in different ratios. Only the equilibrium situation has been considered. An explanation has been given for the difference in the melting temperatures of dAT:dAT and dA:dT. Exact calculations have been made for the average fraction of hydrogen bonds intact at a particular temperature assuming that the correlation between nearest neighbor hydrogen bonds is independent of the nature of the bond. A linear variation of

melting temperature with the concentration of GC (or AT) bonds has been found, agreeing with the available experimental data. The calculated variation of the slope of the melting curve with respect to GC concentration agrees qualitatively with the observed one. The third model has been extended up to three nearest neighbor correlations assuming exponential decrease of correlation. Variation of the width of the transition with pH agrees qualitatively with the experiments. Procedures for the extension of the calculations to the general case of correlation dependent on the nature of the hydrogen bond have been formulated.

It is planned to study the kinetics using both the zipper and modified Ising models under less restricted conditions, especially in the light of recent experimental work.

(E) Research investigations in human learning and statistical analysis of research data

Principal investigator

Dr. Nancy Anderson	Associate Professor	Psychology

Project No.	Initiated	Completed	Computer time* Reporting period	Computer time* Total
206/64/024	8/64	In progress	0/23	0/23

Objectives:

Recent research has emphasized that the influence of interference on short term retention is analogous to that found in long term retention. Since there is evidence that variables influence retention, be the test intervals long or short, in the same or similar manner, it has been concluded that the retention processes are the same. Recent studies have been conducted using an acoustic similarity variable which showed that the effects are opposite on short term retention as compared to long term retention, when letters of the alphabet are used in a task requiring serial reproduction. In this case the influence of acoustic similarity differentially affected short and long term retention. The implications of these results for theories of short and long term retention will be studied.

*Only time used since September 1965 is given here.

(F) Predictive mathematical models for performance on operant conditioning schedules

Candidate: R. M. Lee — Psychology
Degree: Ph.D.

Principal advisor: Dr. Nancy Anderson

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
206/64/003	4/64	In progress	2/21	4/31

(G) Effect of violation of assumptions on the t-test of significance of intercorrelations

Candidate: R. N. Harris — Psychology
Degree: Ph.D.

Principal advisor: Dr. E. I. Heerman

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
206/65/043	5/65	1/66	0	0

Results:

A doctoral dissertation entitled "Multiple Significance Tests of Correlation Coefficients in Correlation Matrices" has been successfully completed as a result of this work.

6. Other computer-oriented research in engineering

This section includes data on eleven projects in the fields of Aerospace, Civil, Electrical and Mechanical Engineering. Information on two additional projects in Electrical Engineering, completed during the first half of 1965, was given in the Semi-annual Status Report.

New projects

305/65/019	Cylindrical "volume" phase delayed antenna arrays
301/65/010	The investigation of the thermal stresses in a conical radome by the method of finite differences

Continuing projects

304/65/003	Analysis of continuous rectangular ortho-tropic plates
305/64/009	UHF propagation prediction analysis and field strength calculations
305/64/008	Construction of a computer design language translator
306/64/001	Upper and lower bounds for the torsional rigidity of solid cylinders of irregular cross-sections
306/63/001	Response functions

Completed projects

305/65/018	Calculation of the reliability of redundant logic networks
306/65/002	Effectiveness of anisotropic rectangular cooling fins
305/65/017	Near field of antenna
305/64/001,5	Coordinate conversion in the omega radio navigation system

(A) Cylindrical "volume" phase delayed antenna arrays

Candidate: Russell Glock, Jr. Electrical
Degree: M. S. Engineering

Principal advisor: Dr. T. C. Wagner

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
305/65/019	9/65	In progress	0/18	0/18

Many antenna systems are being used today which make use of electronic phase delay to steer the antenna. One such antenna is a cylindrical "volume" antenna array in which elementary elements are placed uniformly throughout a volume of space having a cylindrical shape.

The solution of the equations for the directivity index and the pattern for such an antenna requires the use of Bessel functions, including a double integration of a function involving a Bessel function. Thus a high speed computer is needed to evaluate these functions.

(B) The investigation of the thermal stresses in a conical radome by the method of finite differences

Candidate: Roger Weiss — Aerospace Engineering
Degree: M. S.

Principal advisor: Dr. Robert Rivello

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
301/65/010	9/65	In progress	0/19	0/19

The thermal stresses in radomes are an important factor in high speed vehicle design. Ceramic materials used in radome construction, while being very strong in compression, are relatively weak in tension. As a result, the analysis of the thermal stresses produced by aerodynamic environments is necessary to insure structural integrity.

This project will determine the thermal stresses in a Pyroceram conical radome resulting from a time-invariant axisymmetric thermal load. The differential equations and boundary conditions describing the physical situation have been written in a finite difference form. By applying the difference scheme of the governing equations at so-called grid points in the conical domain, a system of simultaneous linear algebraic equations results. The number of equations which results depends upon the size of the grid spacing, i.e. upon how finely the conical domain is sub-divided. However, to obtain the solutions to the problem, involving 172 equations, it is necessary to employ high speed computer techniques.

(C) Analysis of continuous rectangular orthotropic plates

Candidate: Conrad P. Heins — Civil Engineering
Degree: Ph.D.

Principal advisor: Dr. Charles T. G. Looney

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
304/65/003	7/65	In progress	1/29	1/29

Interim results:

Many new bridge structures are being designed so that the steel deck plate and stiffening members act as a unit. This type of system produces economy of material as well as structural soundness. However, in order to properly design such a structure, a suitable method of analysis is necessary. The method being developed on this project will enable a designer to investigate such complex structures, designated as "orthotropic bridges".

Two methods of solving an orthotropic plate on flexible supports have been developed. Both techniques involve the solution of the bi-harmonic plate differential equation, as applied to the boundary conditions of a bridge structure. One uses finite differences, the other a trigonometric series solution.

The finite differences method involves the solution of simultaneous equations. The Gauss Substitution Technique will be employed after the matrix is established. In the trigonometric series solution, by approximating the external forces in a Fourier Series format, the sum of each component is determined and summed up at each desired location.

(D) UHF propagation prediction analysis and field strength calculations

Principal investigator

Mr. J. V. Larson	Instructor	Electrical Engineering

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
305/65/009	10/64	In progress	2/27	4/41

Interim results:

Thus far programs have been developed to obtain far field patterns for antenna arrays and directive antennas at elevated heights above a smooth non-perfect reflecting surface. These programs have been tested and seem to give satisfactory results.

The future plans for the project are to use these programs to generate data for a number of different values of the parameters involved. These data would then be analyzed and plotted. The resulting curves will hopefully be useful in gaining more insight to the problems involved, and may also be useful as design criteria for communications system designers.

Extensive use of the CALCOMP plotter is anticipated.

(E) Construction of a computer design language translator

Principal investigator

Dr. Yaohan Chu	Professor	Electrical Engineering

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
305/64/008	7/64	In progress	0	0

(F) Upper and lower bounds for the torsional rigidity of solid cylinders of irregular cross-sections

Principal investigator

Dr. J. C. S. Yang	Assistant Professor	Mechanical Engineering

			Computer time	
Project No.	Initiated	Completed	Reporting period	Total
306/64/001	7/64	In progress	0/39	1/55

(G) Response functions

Principal investigator

Dr. B. S. Berger — Assistant Professor — Mechanical Engineering

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
306/63/001	9/63	In progress	0/7	0/52

Interim results:

Multiple integral transforms - Laplace-Fourier, Laplace-Hankel, n-dimensional Laplace and n-dimensional Fourier - have proven to be of considerable value in the analysis of the response of elastic bodies [1,2,3]. The computation of the integral transform of the solution and the calculation of the inverse of the transform of the solution are fundamental problems arising from the application of integral transforms to the systems of partial differential equations encountered in the vibration of elastic bodies.

This investigator has resolved the problem of the inversion of the multiple Laplace transform in terms of an n-series of ultraspherical polynomials. It is probable that further generalizations are possible which will lead to more rapidly converging series. The computer facility will be necessary in the evaluation of coefficients occurring in the expansions and in the numerical determination of the convergence characteristics of the series.

Expressions for the transforms of the dynamic responses of thin plates of various shapes and cylindrical shells have been derived by the investigator. These results together with the series solutions to the inversion problem will be used in the solution of the dynamic response of a technically interesting class of elastic systems consisting of interconnected beams, plates and shells. It is anticipated that various examples will be solved numerically as a verification of the validity of the expressions derived for the transforms and as a test of the practicality of the method.

References

[1] Voelker, D. and G. Doetsch, Die zweidimensionale Laplace-transformation, Verlag Birkhäuser, Basel, 1950

[2] Nigul, V. K., The application of the three-dimensional theory of elasticity to the analysis of flexural waves in a semi-infinite plate acted on by a short-time boundary loading, P.M.M. Vol. 27, No. 6, 1963, pp. 1044-1056

[3] Eason, G., On the torsional impulsive loading of an elastic half space, Quart. Journ. Mech. & Appl. Math., Vol. XVII, Pt. 3, 1964

(H) Calculation of the reliability of redundant logic networks

Candidate: R. E. Lyons — Electrical Engineering
Degree: Ph.D.

Principal advisor: Dr. Alan B. Marcovitz

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
305/65/018	7/65	1/66	1/0	1/0

Computational work on this project is completed; the dissertation is in preparation.

(I) Effectiveness of anisotropic rectangular cooling fins

Candidate: L. C. Taylor — Mechanical Engineering
Degree: M. S.

Principal advisor: Dr. R. W. Allan

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
306/65/002	3/65	1/66	0/42	0/42

Results:

A thesis entitled "Heat Conduction in Anisotropic Fins" is now being prepared. An analysis is presented of the steady temperature fields in convectively cooled (constant h) anisotropic longitudinal fins (constant k) of rectangular cross section and circumferential fins of rectangular cross section. The fin effectiveness is determined over a range of anisotropicity up to $k_x/k_y = 10{,}000$.

Factors are obtained which show the ratio between circumferential fin effectiveness and longitudinal fin effectiveness. It is shown how the problem of the rectangular fin with anisotropicity along principal axes relates to the standard fin with different unit surface conductances on tip and sides. Numerical effectivenesses are presented on fine-grid charts over a wide range of parameters.

(J) Near field of antenna

Candidate: D. L. Hipkins — Electrical Engineering
Degree: M. S.

Principal advisor: H. R. Reed

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
305/65/017	2/65	1/66	13/55	13/55

(K) Coordinate conversion in the omega radio navigation

Candidate: M. M. Smith — Electrical Engineering
Degree: M. S.

Principal advisor: Dr. Alan Marcovitz

Project No.	Initiated	Completed	Computer time: Reporting period	Computer time: Total
305/64/001,5	1/64	9/65	0/25	5/23

Mr. Smith has left the University without obtaining significant results in the area of this project.

Appendix 1

COMPUTER TIME SUMMARY
Recorded Time* by College
February, 1965 - July, 1965

	Feb.	Mar.	Apr.	May	June	July	Total
I. Academic Use (Execution time only)							
Computer Science Center	83	92	95	134	181	156	741
College of Arts & Sciences	127	181	197	124	110	135	874
College of Engineering	7	48	38	41	26	24	184
College of Business & Public Administration	8	14	17	16	8	10	73
College of Agriculture**	10	15	12	9	16	13	75
College of Education		1	4	3	3	3	14
School of Medicine	2	3	5	7	6	4	27
Other Units of the University				2		3	5
Cooperative Research with other Educational Institutions	5	4	2	3	6	7	27
II. Computer Maintenance	42	58	56	49	50	30	285
III. Set-up Time***	39	44	42	57	47	41	270
TOTAL	323	460	468	445	453	426	2575
OTHER TIME (including idle and unreported)	213	190	125	170	151	153	1002
CONSOLE LOG ON-TIME	536	650	593	615	604	579	3577

* Rounded to next full hour
** Includes Natural Resources Institute
*** Time consumed before and after runs involving executive and subsystems in control, the appropriate monitors, and required operator activity.

Appendix 1 (Cont'd.)

COMPUTER TIME SUMMARY
Recorded Time* by College
August, 1965 - January, 1966

	Aug.	Sept.	Oct.	Nov.	Dec.	Jan.	Total
I. Academic Use (Execution time only)							
Computer Science Center	120	140	54	58	61	64	497
College of Arts & Sciences	169	138	158	153	135	142	895
College of Engineering	21	19	38	24	21	32	155
College of Business & Public Administration	12	11	22	24	17	24	110
College of Agriculture**	18	11	18	12	18	8	85
College of Education	7	1	1	1	1	2	13
School of Medicine	10	5	5	7	6	9	42
Other Units of the University	10	4	2	2	4	4	26
Cooperative Research with other Educational Institutions	8	4	6	6	5	10	39
II. Computer Maintenance	39	42	34	28	31	18	192
III. Set-up Time***	80	98	69	46	36	42	371
TOTAL	494	473	407	361	335	355	2425
OTHER TIME (Including idle and unreported)	161	140	218	234	218	231	1203
CONSOLE LOG ON-TIME	655	613	625	595	553	586	3627

* Rounded to next full hour
** Includes Natural Resources Institute
*** Time consumed before and after runs involving executive and subsystems in control, the appropriate monitors, and required operator activity.

Appendix 2

TABLE OF COMPUTER TIME USED BY PROJECTS RECEIVING COMPUTATIONAL SUPPORT UNDER NASA GRANT NsG 398*

February, 1965 - July, 1965

	Feb.	Mar.	Apr.	May	June	July	Total
Computer Science Center							
Programming Systems	12	16	13	16	23	17	97
Numerical Mathematics	11	4	4	3	14	7	43
Image Processing	5	8	8	6	5	12	44
College of Arts and Sciences							
Chemistry	22	26	22	40	16	6	132
Other Departments	10	10	9	17	10	28	84
College of Engineering	5	37	15	22	24	18	121
TOTAL	65	101	71	104	92	88	521
% Supported by Grant NsG 398	49%	41%	54%	40%	45%	47%	45%
Total Time Supported by NsG 398	32	41	38	42	41	41	235

*Usage is shown to the nearest hour.

Appendix 2
(Cont'd.)

TABLE OF COMPUTER TIME USED BY PROJECTS RECEIVING COMPUTATIONAL SUPPORT UNDER NASA GRANT NsG 398*

August, 1965 - January, 1966

	Aug.	Sept.	Oct.	Nov.	Dec.	Jan.	Total
Computer Science Center							
Programming Systems	10	13	9	10	10	10	62
Numerical Mathematics	6	4	6	3	1	4	24
Image Processing	10	10	3	5	2	2	32
College of Arts and Sciences							
Chemistry	26	30	28	19	22	32	157
Other Departments	16	20	16	9	12	8	81
College of Engineering	13	17	30	19	12	18	109
TOTAL	81	94	92	65	59	74	465
% Supported by Grant NsG 398	49%	45%	45%	65%	71%	57%	53%
Total Time Supported by NsG 398	40	42	41	42	42	42	249

*Usage is shown to the nearest hour.

APPENDIX 3. PUBLICATIONS, REPORTS AND THESES

(A) TECHNICAL REPORTS OF THE COMPUTER SCIENCE CENTER

1. TECHNICAL NOTE TN-63-1
NSG-398 SEPTEMBER 1963
SINKOV, ABRAHAM. "A COMPUTER APPLICATION TO GROUP THEORY." COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

2. TECHNICAL REPORT TR-63-2
NSG-398 OCTOBER 1963
KURODA, SIGEKATU AND JOHN MARYAK. "ON SIEVES AND PRIMES." DEPARTMENT OF MATHEMATICS, UNIVERSITY OF MARYLAND.

3. TECHNICAL REPORT TR-63-3
NSG-398 OCTOBER 1963
BEAM, ALFRED E. "MULTIPLE PRECISION PACKAGE, UOM MPP FOR THE IBM 7090/7094." COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

4. TECHNICAL REPORT TR-63-4
NSG-398 NOVEMBER 1963
SNIVELY, JAMES W. "THE USE OF DIGITAL COMPUTERS TO DETERMINE DEFINITIONS FOR ABSTRACT GROUPS." COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

5. TECHNICAL REPORT TR-64-5
NSG-398 JANUARY 1964
BERNS, GERALD M. "MOIST (MACRO OUTPUT INPUT SYSTEM FOR THE IBM 7090)." IBM CORPORATION.

6. TECHNICAL REPORT TR-64-6
NSG-398 APRIL 1964
STEWART, JAMES, "CRYSTAL STRUCTURE CALCULATIONS SYSTEM, X-RAY - '63, FOR THE IBM 709/7090/7094." COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND AND RESEARCH COMPUTER CENTER, UNIVERSITY OF WASHINGTON.

7. TECHNICAL REPORT TR-64-7
NSG-398 MAY 1964
LINDAMOOD, GEORGE E. "NUMERICAL ANALYSIS IN RESIDUE NUMBER SYSTEMS." COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

8. TECHNICAL REPORT TR-64-8
NSG-398 JUNE 1964
ANDERSON, NANCY S., AZRIEL ROSENFELD, AND NORMAN F. SIMENSON. ''PATTERN RECOGNITION - I. A COMPUTER PROGRAM FOR GENERATING SYNTHETIC PATTERNS.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

9. TECHNICAL REPORT TR-64-9
NSG-398 JUNE 1964
BERNS, GERALD M. ''UTILIZING THE MACRO GENERATOR OF IBMAP FOR THE IBM 7090/7094.'' IBM CORPORATION.

10. TECHNICAL REPORT TR-64-10
NSG-398 AUGUST 1964
CRTON, JAMES N. AND AZRIEL ROSENFELD. ''PATTERN RECOGNITION - II. RAMP AND REST, TWO IMAGE ANALYSIS PROGRAMS.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

11. TECHNICAL REPORT TR-64-11
NSG-398 OCTOBER 1964
FITZWATER, DONALD R. AND EARL J. SCHWEPPE. ''CONSEQUENT PROCEDURES IN CONVENTIONAL COMPUTERS.'' INSTITUTE FOR ATOMIC RESEARCH AND DEPARTMENT OF CHEMISTRY, IOWA STATE UNIVERSITY AND COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

12. TECHNICAL REPORT TR-64-12
NSG-398 DECEMBER 1964
ORTEGA, JAMES M. ''THE GIVENS-HOUSEHOLDER METHOD FOR SYMMETRIC EIGENVALUE PROBLEM.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

13. TECHNICAL REPORT TR-65-13
NSG-398 JANUARY 1965
ORTON, JAMES N. AND AZRIEL ROSENFELD. ''PATTERN RECOGNITION - III. SORD-1 AND SORD-2. TWO PROGRAMS FOR DELINEATING 'SOLID' AND 'BROKEN' REGIONS IN AN IMAGE.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

14. TECHNICAL REPORT TR-65-14
NSG-398 FEBRUARY 1965
RHEINBOLDT, WERNER C. ''ON A GENERAL ESTIMATION PRINCIPLE AND A THEORY OF COMPARISON-FACTORS.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

15. TECHNICAL REPORT TR-65-15
NSG-398 APRIL 1965
BEAM, ALFRED E. ''MAMOS- A MONITOR SYSTEM UNDER IBSYS FOR THE IBM 7090/7094.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

16. TECHNICAL REPORT TR-65-16
NSG-398 MAY 1965
ORTEGA, JAMES N. AND WERNER C. RHEINBOLT. ''ON DISCRETIZATION AND DIFFERENTIATION OF OPERATORS WITH APPLICATION TO NEWTON'S METHOD.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

17. TECHNICAL NOTE TN-65-17
NSG-398 APRIL 1965
WACTLAR, HOWARD D. ''THE UNIVERSITY OF MARYLAND 1401 TRANSLITERATION PREPROCESSOR FOR ALGOL 60 TO ALCOR-ILLINOIS 7090/94 CONVERSION.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

18. TECHNICAL REPORT TR-65-18
NSG-398 MAY 1965
ROSENFELD, AZRIEL AND JOHN L. PFALTZ. ''PATTERN RECOGNITION- IV. SEQUENTIAL OPERATIONS IN DIGITAL PICTURE PROCESSING.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

19. TECHNICAL REPORT TR-65-19
NSG-398 JUNE 1965
WILLIAMS, JAMES F. ''AN EMPIRICAL EVALUATION OF LATENT CLASS ANALYSIS.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

20. TECHNICAL REPORT TR-65-20
NSG-398 AUGUST 1965
ORTEGA, JAMES M. AND MAXINE L. ROCKOFF, ''NON-LINEAR DIFFERENCE EQUATIONS AND GAUSS-SEIDEL TYPE ITERATIVE METHODS.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

21. TECHNICAL REPORT TR-65-21
NSG-398 AUGUST 1965
MONMONIER, MARK S., JOHN L. PFALTZ AND AZRIEL ROSENFELD. ''PATTERN RECOGNITION- V. SAMP- A COMPUTER PROGRAM FOR ESTIMATING SURFACE AREA FROM CONTOUR MAPS.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

22. TECHNICAL REPORT TR-65-22
NSG-398 AUGUST 1965
WACTLAR, HOWARD D. ''PAPER TAPE CONVERSION PROCEDURES.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

23. TECHNICAL REPORT TR-65-23
NSG-398 SEPTEMBER 1965
PFALTZ, JOHN L. ''TREETRAN- A FORTRAN IV SUBROUTINE PACKAGE FOR MANIPULATION OF ROOTED TREES.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

24. TECHNICAL REPORT TR-65-24
NSG-398 OCTOBER 1965
PARK, CHAN M. ''SUBROUTINES FOR DIGITAL COMPUTATION OF CHEMICAL ENGINEERING PROBLEMS.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

25. TECHNICAL REPORT TR-65-25
NSG-398 NOVEMBER 1965
EASTLAKE, DONALD E. ''FORTRAN II TO FORTRAN IV TRANSLATOR.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

26. TECHNICAL REPORT TR-66-26
NSG-398 JANUARY 1966
BEAM, ALFRED E. ''INPUT-OUTPUT SUBROUTINE PACKAGE FOR THE IBM 7090/7094.'' COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND.

(B) OTHER REPORTS AND PUBLICATIONS

ARMSTRONG, J.C., M.J. BAGGETT, W.R. HARRIS AND V.A. LATORRE
"THE 1.7-MEV ANOMALY IN THE C(12)(P,P) C(12) REACTION."
DEPARTMENT OF PHYSICS AND ASTRONOMY, TECHNICAL REPORT 488.1965.14 PP.

ATKINSON, GORDON AND SUSHIL K. KOR
"KINETICS OF ION ASSOCIATION IN MNSO4 SOLUTIONS I. RESULTS IN WATER DIOXANE AND METHANOL WATER MIXTURES AT 25 DEGREES C."
JOURNAL OF PHYSICAL CHEMISTRY, VOL. 69. 1965. P. 164.

ATKINSON, GORDON AND SUSHIL K. KOR
"CONDUCTANCE OF CUBDS AND SRBDS IN METHANOL-WATER AND ACETONE-WATER MIXTURES AT 25 DEGREES C."
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY, VOL. 87. 1965. P. 164.

BEAM, ALFRED
"MULTIPLE-PRECISION PACKAGE WITH I/O."
SHARE DISTRIBUTION MS3081 ALY UOM-MPP, COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND. 1964.

BEAM, ALFRED
"USE OF IBM BASIC MONITOR (IBSYS) AND ASSOCIATED SYSTEMS."
COMPUTER SCIENCE CENTER, UNIVERSITY OF MARYLAND. 1963. 61 P.

BENESCH, WILLIAM M. AND JOSEPH T. VANDERSLICE
"POTENTIAL CURVES FOR THE OBSERVED STATES OF N(2) BELOW 11 E.V."
ACCEPTED FOR PUBLICATION IN THE ASTROPHYSICAL JOURNAL.

BENESCH, WILLIAM M. AND JOSEPH T. VANDERSLICE
"FRANCK-CONDON FACTORS IN OBSERVED TRANSITIONS IN N(2) ABOVE 6 E.V."
ACCEPTED FOR PUBLICATION IN THE ASTROPHYSICAL JOURNAL.

BERGER, BRUCE S.
"DYNAMIC RESPONSE FUNCTIONS."
JOURNAL OF THE ENGINEERING MECHANICS DIVISION, AMERICAN SOCIETY OF CIVIL ENGINEERING, 90, EM4, AUGUST, 1964. PP. 131-147.

BETTINGER, ROBERT T.
"AN IN-SITU PROBE SYSTEM FOR THE MEASUREMENT OF IONOSPHERIC PARAMETERS."
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 277. 1964.

CRONYN,W.M. AND W.C. ERICKSON
"THE FLUX AND BRIGHTNESS DISTRIBUTION OF THE SUN AT 26.3MC/SEC."
PAPER PRESENTED AT THE 119TH MEETING OF THE AMERICAN ASTRONOMICAL SOCIETY, HELD 3-6 AUGUST 1965 AT THE UNIVERSITY OF MICHIGAN, ANN ARBOR, MICHIGAN.

DAVIES, ROBIN H. AND JOSEPH T. VANDERSLICE
''VALIDITY OF THE JARMAIN- SANDEMAN SERIES FOR CALCULATING POTENTIAL CURVES OF DIATOMIC MOLECULES.''
ACCEPTED FOR PUBLICATION IN THE CANADIAN JOURNAL OF PHYSICS.

DAVIES, ROBIN H., E.A. MASON, AND R.J. MUNN
''HIGH-TEMPERATURE TRANSPORT PROPERTIES OF ALKALI METAL VAPORS.''
PHYSICS OF FLUIDS, VOL. 8. 1965. P. 444.

DEROCCO, ANDREW G.
''INTERMOLECULAR FORCES, THE TRIANGLE WELL AND SOME COMPARISONS WITH THE SQUARE WELL.''
JOURNAL OF CHEMICAL PHYSICS, VOL. 41. 1964.

DETENBECK, ROBERT W., JERRY B. MARION., ET. AL.
''TRANSFORMATION TABLES BETWEEN LABORATORY AND CENTER OF MASS COORDINATES FOR CALCULATIONS OF ENERGIES OF REACTION PRODUCTS.''
OAK RIDGE NUCLEAR LABORATORY REPORT 2574. 1964.

DETENBECK, ROBERT W.
''UNSCRAMBLING PULSE-HEIGHT SPECTRA ONLINE.''
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 362. 1964. ALSO INSTITUTE OF ELECTRICAL AND ELECTRONICS ENGINEERS TRANSACTIONS ON NUCLEAR SCIENCE, NS-11. 1964. P. 344.

FALLER, ALAN J.
''LARGE EDDIES IN THE ATMOSPHERIC BOUNDARY LAYER AND THEIR POSSIBLE ROLE IN THE FORMATION OF CLOUD ROWS.''
JOURNAL OF THE ATMOSPHERIC SCIENCES, VOLUME 22. 1965. PP. 176-184.

FALLER, ALAN J. AND ROBERT E. KAYLOR
''A NUMERICAL STUDY OF THE INSTABILITY OF THE LAMINAR EKMAN BOUNDARY LAYER.''
INSTITUTE FOR FLUID DYNAMICS AND APPLIED MATHEMATICS, UNIVERSITY OF MARYLAND, TECHNICAL NOTE BN-410. 1965. 25 PP.

FANN, HUGO L.
''THE POLARIZATION OF PROTONS FROM THE HE(3)(D,P)HE(4) REACTION.''
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 376. 1964.

FITZWATER, D. R. AND EARL J. SCHWEPPE
''CONSEQUENT PROCEDURES IN CONVENTIONAL COMPUTERS.''
PROCEEDINGS OF THE AMERICAN FEDERATION OF INFORMATION PROCESSING SOCIETIES CONFERENCE, SAN FRANCISCO, CALIFORNIA. OCTOBER 1964.

FORSYTH, P.D., A.R. KNUDSON AND F.C. YOUNG
''A SEARCH FOR THE 5.58 AND 6.40 MEV EXCITED STATES OF B(10).''
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 515. 1965.

FRIED, C., A. ROSENFELD AND L. J. GERSTMAN
''SEQUENTIAL AND PARALLEL PROCESSING IN BOUNDARY SELECTIONS ON ONE-DIMENSIONAL PICTORIAL STIMULI.''
PERCEPTUAL AND MOTOR SKILLS, VOL. 20. 1965. PP. 789-801.

GOLDSTEIN, A. AND AZRIEL ROSENFELD
''SYSTEMS FOR GENERATING ONE DIMENSIONAL PATTERNS.''
APPLIED OPTICS, VOL. 3. 1964. PP. 547-548.

GOMEZPLATA, A. AND R.W. BROWN
''PROBLEMS IN REACTOR DESIGN.''
DEPARTMENT OF CHEMICAL ENGINEERING, TECHNICAL REPORT.1965. 32 PP.

GORDON, GILBERT AND A. ANDREWES
''THE OXIDATION OF AQUEOUS URANIUM (IV) BY BROMINE.''
INORGANIC CHEMISTRY, VOL. 3. 1965. P. 1732.

GORDON, GILBERT AND BASSAM Z. SHAKHASHIRI
''THE HETEROGENEOUS EXCHANGE REACTION BETWEEN GASEOUS OXYGEN AND VARIOUS OXYGEN-CONTAINING SALTS.''
JOURNAL OF INORGANIC AND NUCLEAR CHEMISTRY. 1965.

GORDON, GILBERT AND P.H. TEWARI
''KINETICS OF THE VANADIUM(II) - CHLORATE REACTION.''
JOURNAL OF PHYSICAL CHEMISTRY. 1965.

HAIGHT, G. P., E. PERCHONOCK, F. P. EMMENEGGER AND G. GORDON
''THE MECHANISM OF THE OXIDATION OF SULFUR(IV) BY CHROMIUM(VI) IN ACID SOLUTION.''
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. 1965.

HIGH, DORIS, R. ALDEN AND J. STEWART
''THE SYMMETRY HANDLING ALGORITHM OF X-RAY 1963.''
PRESENTED AT THE ANNUAL MEETING OF THE AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, BOZEMAN, MONTANA, JULY 1964.

HIRST, L.L. AND R.E. PRANGE
''EXCHANGE EFFECTS IN FERROMAGNETIC RESONANCE WITH NONLOCAL CONDUCTIVITY.''
THE PHYSICAL REVIEW, VOL. 139. NO. 3A. A892-A900. 1965.

KACSER, CLAUDE AND I.J.R. AITCHISON
''APPARENT, BUT ENERGY-DEPENDENT PSEUDO-RESONANCES DUE TO RE-SCATTERING IN SEQUENTIAL PROCESSES.''
REVIEWS OF MODERN PHYSICS, VOL 37. NO. 3. 1965. PP. 350-354.

LATORRE, V.A. AND J.C. ARMSTRONG
''N(14) LEVELS FROM ELASTIC SCATTERING OF PROTONS BY C(13).''
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 495, 1965. 32PP.

LATORRE, VICTOR A.
"ELASTIC SCATTERING OF PROTONS FROM C12 AND C13."
BULLETIN OF THE AMERICAN PHYSICAL SOCIETY, VOL. 9. 1964. P. 418.

LEE, RICHARD M.
"AN UNCORRELATED SCHEDULE OF REINFORCEMENT WITH TEMPORAL AND FIXED RATIO CONTINGENCIES."
DEPARTMENT OF PSYCHOLOGY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 65-42. 1965.

LIWSHITZ, MORDEHAI AND S.F. SINGER
"THERMAL ESCAPE OF NEUTRAL HYDROGEN AND ITS DISTRIBUTION IN THE EARTH'S THERMOSPHERE."
NASA TECHNICAL NOTE, NASA TN D-2992.1965. 25 PP.

LOEBBAKA, DAVID AND JOGESH PATI
"DYNAMICS AND SYMMETRIES OF NONLEPTONIC HYPERON DECAYS, SCALAR MESON COUPLINGS."
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT NO. 541. 1966.31 PP.

LOEBBAKA, DAVID AND JOGESH PATI
"NORMAL SCALAR NONET, K(1) 2 PI -DECAY AND K(1)-K(2) MASS DIFFERENCE."
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT NO. 511.1965. 30 PP.

LUDEMANN, CARL A., WILLIAM F. HORNYAK AND HARRY D. HOLMGREN
"ANGULAR DISTRIBUTION AND CORRELATIONS IN THE C(12)(HE(3),P)N(14) REACTION."
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 389. 1964.

LUKE, SUIKAY AND STANLEY WEISSMAN
"BESSEL FUNCTIONS OF IMAGINARY ORDER AND IMAGINARY ARGUMENT."
INSTITUTE FOR MOLECULAR PHYSICS, UNIVERSITY OF MARYLAND, TECHNICAL REPORT. AUGUST 1964.

MEIVERS, MICHAEL R.
"BUCKLING OF A TAPERED SHAFT DUE TO COMBINED TORSION AND COMPRESSION."
DEPARTMENT OF AERONAUTICAL ENGINEERING, UNIVERSITY OF MARYLAND, TECHNICAL REPORT. MAY 1964.

MISNER, CHARLES W. AND HAROLD S. ZAPOLSKY
"HIGH DENSITY BEHAVIOR AND DYNAMIC STABILITY OF NEUTRON STAR MODELS."
PHYSICAL REVIEW LETTERS, VOL. 12. NO. 22. JUNE 1964. PP. 635-637.

MISNER, CHARLES W.
"OUTER NUT SPACE."
JOURNAL OF MATHEMATICAL PHYSICS, VOL. 4. NO. 7. 1963.

MOAZED, CYRUS, J.E. ETTER, H.D. HOLMGREN AND M.A. WAGGONER
''THE BE(9) ((HE(3),A))2HE(4) REACTION.''
PHYSICS LETTERS, VOL. 12. 1964. PP. 45-48.

MOAZED, CYRUS, J.E. ETTER, H.D. HOLMGREN AND M.A. WAGGONER
''PARTICLE-PARTICLE ANGULAR CORRELATION FOR THE BE(9) ((HE(3),A)) BE(8)--AA REACTION.''

MOAZED, CYRUS, J.E. ETTER, H.D. HOLMGREN AND M.A. WAGGONER
''THE BE(9) ((HE(3), AAA)) REACTION.''
REVIEWS OF MODERN PHYSICS, VOL 37. NO. 3. 1965. PP. 354-357.

MOAZED, CYRUS, J.E. ETTER, H.D. HOLMGREN, M.A. WAGGONER, AND C. HAN
''SPECTROSOPIC STUDIES WITH THE B(10) ((HE(3), PAAA)) REACTION.''
REVIEWS OF MODERN PHYSICS, VOL 37. NO. 3. 1965. PP. 444-447.

MOAZED, CYRUS, J.E. ETTER, H.D. HOLMGREN, M.A. WAGGONER AND A.A. JAFFE
''THE B(10) ((HE(3), PA))2HE(4) REACTION).''
PHYSICS LETTERS, VOL. 12. NO. 1. 1964. PP. 42-45.

MOAZED, C., J.E. ETTER, H.D. HOLMGREN AND M.A. WAGGONER
''THE BE(10) ((HE(3), PAAA)) REACTION PROCESS.''
REVIEWS OF MODERN PHYSICS, VOL. 37. NO. 3. 1965. PP. 444-447

MONMONIER, MARK S.
''THE PRODUCTION OF SHADED MAPS ON THE DIGITAL COMPUTER.''
THE PROFESSIONAL GEOGRAPHER,VOL. 17. NO. 5. 1965. PP 13-14.

MONTROLL, ELLIOTT AND NARENDRA GOEL
''DENATURATION AND RENATURATION OF DNA. I EQUILIBRIUM STATISTICS OF COPOLYMERIC DNA.''
INSTUTUTE FOR FLUID DYNAMICS AND APPLIED MATHEMATICS, UNIVERSITY OF MARYLAND, TECHNICAL NOTE BN-425. 1965. 29 PP.

MUNN, ROBERT J. AND FRANCIS J. SMITH
''INTERACTION POTENTIAL OF THE INERT GASES. II.''
INSTITUTE FOR MOLECULAR PHYSICS, UNIVERSITY OF MARYLAND,IMP-NASA-47. 1965.

MUNN, ROBERT J., EDWARD A. MASON AND FRANCIS J. SMITH
''TRANSPORT PROPERTIES OF GASEOUS HE(3) AND HE(4).''
ACCEPTED FOR PUBLICATION IN THE PHYSICAL REVIEW.

MUNN, ROBERT J., EDWARD A. MASON AND FRANCIS J. SMITH
''COLLISION INTEGRALS FOR THE EXPONENTIAL ATTRACTIVE POTENTIAL.''
PHYSICS OF FLUIDS, VOL. 8. 1965. P. 1103.

MUNN, ROBERT J., EDWARD A. MASON AND FRANCIS J. SMITH
''SOME ASPECTS OF THE QUANTAL AND SEMICLASSICAL CALCULATION OF PHASE SHIFTS AND CROSS SECTIONS FOR MOLECULAR SCATTERING AND TRANSPORT.''
JOURNAL OF CHEMICAL PHYSICS, VOL. 41. NO. 12. 1964. PP. 3978-3988.

MUNN, ROBERT J., EDWARD A. MASON, FRANCIS J. SMITH AND L. MONCHIK
''TRANSPORT COLLISION INTEGRALS FOR QUANTUM GASES OBEYING A 12-6 POTENTIAL.''
JOURNAL OF CHEMICAL PHYSICS, VOL. 42 1965. PP. 1334-1339.

ONEDA, SADAO, Y.S. KIM AND L.M. KAPLAN
''FINAL-STATE INTERACTIONS IN N(O)--3 PI DECAY.''
NUOVO CIMENTO, VOL. 34. 1964. PP. 655-664.

PATI, JOGESH C.
''DYNAMICAL MODEL OF THE 1535 MEV XI*-HYPERON.''
PHYSICAL REVIEW, B387. 1964. P. 134.

PATI, JOGESH C. AND DAVID LOEBBAKA
''ABNORMAL QUANTUM NUMBER AND DECAY CHANNELS, J(PG) ASSIGNMENT FOR EPSILON, A NORMAL SCALAR OCTET.''
PHYSICAL REVIEW LETTERS, 14. 1965. P. 929.

RHEINBOLDT, WERNER C.
''ON THE COMPARISON FACTOR IN APPROXIMATION PROBLEMS.''
PRESENTED AT THE MEETING ON FUNCTIONAL ANALYTIC METHODS IN NUMERICAL MATHEMATICS, MATHEMATICS RESEARCH INSTITUTE, OBERWOLFACH/GERMANY. JUNE 1964.

ROOS, PHILIP G. AND N.S. WALL
''THE ELASTIC SCATTERING OF 160 MEV PROTONS FROM BE(9), CA(40), NI(58), SN(120) AND PB(208).''
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 475. 1965.

ROSENFELD, AZRIEL
''ON MODELS FOR THE PERCEPTION OF VISUAL TEXTURE.''
PROCEEDINGS OF THE SYMPOSIUM ON MODELS FOR THE PERCEPTION OF SPEECH AND VISUAL FORM. 1965.

ROSENFELD, AZRIEL, C. FRIED AND J. N. ORTON
''AN APPROACH TO THE AUTOMATIC INTERPRETATION OF CLOUD COVER PICTURES.''
PHOTOGRAMMETRIC ENGINEERING, VOL. 31. 1965.

ROSENFELD, AZRIEL
''AUTOMATIC RECOGNITION OF PICTORIAL FORM.''
PRESENTED AT THE SYMPOSIUM ON AUTOMATIC RECOGNITION OF FORM, ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE, 131ST ANNUAL MEETING, MONTREAL, CANADA. DECEMBER 1964.

ROSENFELD, AZRIEL
''PERCEPTRONS AS 'FIGURE' DETECTORS.''
INSTITUTE OF ELECTRICAL AND ELECTRONICS ENGINEERS TRANSACTIONS ON INFORMATION THEORY, IT-11. 1965.

ROSENFELD, AZRIEL
"AUTOMATIC IMAGERY INTERPRETATION."
PHOTOGRAMMETRIC ENGINEERING, VOL. 31. 1965. PP. 240-242.

ROSENFELD, AZRIEL
"GEOMETRICAL PROBABILITY IN AUTOMATIC PATTERN RECOGNITION."
PROCEEDINGS OF THE INSTITUTE OF ELECTRICAL AND ELECTRONICS ENGINEERS, VOL. 52. 1964. PP. 1269-1270.

ROSENFELD, AZRIEL AND A. GOLDSTEIN
"OPTICAL CORRELATION FOR TERRAIN TYPE DISCRIMINATION."
PHOTOGRAMMETRIC ENGINEERING, VOL. 30. 1964. PP. 639-646.

ROSENFELD, AZRIEL, CHARLES FRIED AND JAMES N. ORTON
"AUTOMATIC CLOUD INTERPRETATION."
PHOTOGRAMMETRIC ENGINEERING NOVEMBER 1965, PP. 991-1002

ROUSH, M. L., M. A. WILSON AND W. F. HORNYAK
"PULSE SHAPE DISCRIMINATION."
NUCLEAR INSTRUMENTATION AND METHODS, VOL. 31. 1964. PP. 112-124.

SHERWOOD, ALBERT E. AND EDWARD A. MASON
"VIRIAL COEFFICIENTS FOR THE EXPONENTIAL REPULSIVE POTENTIAL."
ACCEPTED FOR PUBLICATION IN PHYSICS OF FLUIDS.

SMITH, FRANCIS J.
"AN ALGORITHM FOR SUMMING OF ORTHOGONAL POLYNOMIAL SERIES AND THEIR DERIVATIVES WITH APPLICATIONS TO CURVE FITTING AND INTERPOLATION."
MATHEMATICS OF COMPUTATION, VOL. 19. NO. 89. 1965. PP. 33-36.

SMITH, FRANCIS J., EDWARD A. MASON, AND ROBERT J. MUNN
"CLASSICAL COLLISION INTEGRALS FOR THE REPULSIVE SCREENED COULOMB POTENTIAL."
INSTUTUTE FOR MOLECULAR PHYSICS, UNIVERSITY OF MARYLAND, IMP-NASA-49. 1965.

SMITH, FRANCIS J., EDWARD A. MASON, AND ROBERT J. MUNN
"TRANSPORT COLLISION INTEGRALS FOR GASES OBEYING 9-6 AND 28-7 POTENTIALS."
JOURNAL OF CHEMICAL PHYSICS, VOL. 42. 1965. PP. 537-539.

SMITH, FRANCIS J. AND ROBERT J. MUNN
"AUTOMATIC CALCULATION OF THE TRANSPORT COLLISION INTEGRALS WITH TABLES FOR THE MORSE POTENTIAL."
JOURNAL OF CHEMICAL PHYSICS, VOL. 41. 1964. PP. 3560-3568.

STEWART, JAMES M.
"A UNIFIED SYSTEM FOR DOING THE COMPUTATIONS FOR THE SOLUTION OF CRYSTAL STRUCTURES FROM X-RAY DIFFRACTION DATA."
PRESENTED AT THE AMERICAN ASSOCIATION FOR THE ADVANCEMENT OF SCIENCE, 131ST ANNUAL MEETING, MONTREAL, CANADA. DECEMBER 1964.

STEWART, JAMES, R. ALDEN AND D. HIGH
''THE X-RAY '63 COMPUTING SYSTEM.''
PRESENTED AT THE ANNUAL MEETING OF THE AMERICAN CRYSTALLOGRAPHIC ASSOCIATION, BOZEMAN, MONTANA. JULY 1964.

TOMPKINS, HOWARD E.
''INFORMATION STORAGE AND RETRIEVAL IN DEPTH.''
PRESENTED AT THE ASSOCIATION FOR COMPUTING MACHINERY CHAPTER MEETING, ANN ARBOR, MICHIGAN. JUNE 10, 1964.

TSAO, CHI-KUNG
''NOZZLE FLOW OF FULLY IONIZED PLASMA BASED ON FLUID THEORY.''
JOURNAL OF APPLIED MATHEMATICS AND PHYSICS, ZAMP, SWITZERLAND. 1965.

WAGGONER, M.A. AND A.A. JAFFE
''A STUDY OF THE REACTIONS O(17)((HE(3),A(0))),O(18)((HE(3), A(0))) AND O(18) ((HE(3),A(1))).''
DEPARTMENT OF PHYSICS AND ASTRONOMY, UNIVERSITY OF MARYLAND, TECHNICAL REPORT 423. 1964.

WEISSMAN, STANLEY AND PAUL H. KRUPENIE
''POTENTIAL ENERGY CURVES FOR CO AND CO(+).''
ACCEPTED FOR PUBLICATION IN THE JOURNAL OF CHEMICAL PHYSICS.

WEISSMAN, STANLEY, J. VANDERSLICE, AND R. BATTINO
''NOTE ON THE RECALCULATION OF THE POTENTIAL CURVES FOR THE GROUND STATES OF I2 AND H2.''
JOURNAL OF CHEMICAL PHYSICS, VOL. 39. 1963. P. 2226.

WEISSMAN, STANLEY
''ESTIMATION OF DIFFUSION COEFFICIENTS FROM VISCOSITY DATA, POLAR AND POLYATOMIC MOLECULES.''
JOURNAL OF CHEMICAL PHYSICS, VOL. 40. 1964. P. 3397.

YANG, J.C.S.
''UPPER AND LOWER BOUNDS FOR THE TORSIONAL RIGIDITY OF SOLID CYLINDERS OF GENERAL CROSS-SECTIONS.''
PRESENTED AT THE NINTH MIDWESTERN MECHANICS CONFERENCE, MADISON, WISCONSIN. AUGUST, 1965.

YOUNG, FRANK, K. JAYARAMAN, J. ETTER, H. HOLMGREN AND M. WAGGONER
''THE LI(6) ((HE(3), PAA)) REACTION.''
REVIEWS OF MODERN PHYSICS, VOL 37. NO. 3. 1965. PP. 362-364.

(C) COMPLETED THESIS PROJECTS

AGUILAR, VICTOR LATORRE
"PROTON ELASTIC SCATTERING FROM CARBON-13."
DOCTOR OF PHILOSOPHY, PHYSICS AND ASTRONOMY. 1965.

BARNES, JOHN D.
"THE DIELECTRIC CONSTANT OF SINTERED COMPACTS OF YTTRIUM OXIDE."
MASTER OF SCIENCE, PHYSICS, 1964.

BETTINGER, RICHARD
"AN IN-SITU PROBE SYSTEM FOR THE MEASUREMENT OF IONOSPHERIC PARAMETERS."
DOCTOR OF PHILOSOPHY, PHYSICS, 1964.

CARLSON, FREDERICK P.
"RESOLUTION PARAMETERS WITH STABLE SINGLE FREQUENCY HE-NE LASERS."
MASTER OF SCIENCE, ELECTRICAL ENGINEERING, 1964.

CHEN, CHAO-MEI
"THERMAL RADIATION EFFECTS ON PLANE COUETTE FLOW WITH POROUS WALLS."
MASTER OF SCIENCE, AERONAUTICAL ENGINEERING, 1964.

CRONYN, WILLARD M.
"THE BRIGHTNESS DISTRIBUTION OF THE SUN AT 11 METERS."
MASTER OF SCIENCE, PHYSICS AND ASTRONOMY, 1965.

DOLINSKY, ADRIAN A.
"INVESTIGATION OF THE LENARD-BALESCU EQUATION."
MASTER OF SCIENCE, INSTITUTE FOR FLUID DYNAMICS AND APPLIED MATHEMATICS, 1965.

FANN, HUOO-LONG
"THE POLARIZATION OF PROTONS FROM HE(3)(D,P)HE(4) REACTION."
DOCTOR OF PHILOSOPHY, PHYSICS, 1964.

FISHER, J.R.
"THE UTILIZATION AND EFFECTIVENESS OF LINEAR ARRAYS OF NEUTRON ABSORBER FILLED TUBES AS CONTROL RODS IN WATER MODULATED NUCLEAR REACTORS."
DOCTOR OF PHILOSOPHY, CHEMICAL ENGINEERING, 1965.

GARSIDE, LEONARD
"THE APPROXIMATION OF A UNIFIED THEORY TO ENERGY LEVELS IN O(16)."
DOCTOR OF PHILOSOPHY, PHYSICS, 1965.

LINDAMOOD, GEORGE E.
"ON NUMERICAL ANALYSIS IN MODULAR ARITHMETIC COMPUTERS."
MASTER OF ARTS, MATHEMATICS, 1964.

LIWSHITZ, MORDEHAI
"INVESTIGATION OF THE NEUTRAL HYDROGEN DISTRIBUTION IN THE UPPER ATMOSPHERE BY MEANS OF THE MONTE CARLO METHOD."
DOCTOR OF PHILOSOPHY, PHYSICS, 1964.

LUDEMANN, CARL A.
"ANGULAR DISTRIBUTION LEAST SQUARES FIT."
DOCTOR OF PHILOSOPHY, PHYSICS, 1964.

OH, SIN K.
"UNSTEADY FLOW OVER A FLAT PLATE IN RADIATION GASDYNAMICS."
MASTER OF SCIENCE, ENGINEERING, 1965.

PARK, CHAN M.
"EFFECTIVE THERMAL CONDUCTIVITY IN A PACKED BED."
MASTER OF SCIENCE, CHEMICAL ENGINEERING, 1964.

RICKARD, JAMES J.
"A PILOT STUDY OF GALACTIC STRUCTURE AS DETERMINED BY 21-CM OBSERVATIONS IN THE PERSEUS REGION."
MASTER OF SCIENCE, ASTRONOMY, 1965.

ROUSH, MARVIN
"OPTIMIZATION OF PARAMETERS FOR PULSE-SHAPE DISCRIMINATION."
DOCTOR OF PHILOSOPHY, PHYSICS, 1964.

SCHOOLEY, LARRY C.
"APPROXIMATION OF TRANSFER FUNCTIONS FOR LOW PASS FILTERS."
MASTER OF SCIENCE, ELECTRICAL ENGINEERING, 1965.

SNIVELY, JR., JAMES W.
"COMPUTER ENUMERATION OF FINITE ABSTRACT GROUPS."
MASTER OF ARTS, MATHEMATICS, 1964.

STARK, JOHN D.
"ION ASSOCIATION OF ZINC SULFATE DETERMINED BY ULTRASONIC ABSORPTION."
MASTER OF SCIENCE, CHEMISTRY, 1965.

TSAO, CHI-KUNG
"NOZZLE FLOW OF FULLY IONIZED PLASMA BASED ON FLUID THEORY."
MASTER OF SCIENCE, AERONAUTICAL ENGINEERING, 1964.

VASAVADA, KASHYAP
"PION DEUTERON SCATTERING PERIOD."
DOCTOR OF PHILOSOPHY, PHYSICS, 1964.

WILLIAMS, JAMES F.
"LATENT STRUCTURE ANALYSIS."
MASTER OF SCIENCE, PSYCHOLOGY, 1965.

(D) THESIS PROJECTS IN PROGRESS

BALL, MILLICENT
''R-MATRIX CALCULATION OF CROSS-SECTIONS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

BHATIA, TARLOCHAN
''STUDY OF THE REACTION N(14)(HE(3),A)N(13*)(P+C(12)).''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

CERMAK, JAMES O.
''ENTRY REGION MASS TRANSFER IN AN ANNULUS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

COPELAND, JOSEPH P.
''DIFFUSION MECHANISMS IN ION EXCHANGE.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

CRAMER, STEPHEN D.
''MOMENTUM TRANSFER OF VISCOELASTIC FLUIDS IN SMOOTH WALLED CONDUITS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

DIAZ, AGUSTIN
''REACTIVITY MEASUREMENT OF THE UNIVERSITY OF MARYLAND REACTOR BY MEANS OF STOCHASTIC PROCESSES.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

EBDON, DAVID W.
''ION ASSOCIATION IN POLYVALENT SYMMETRICAL ELECTROLYTES.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

ELLIS, WILLIAM B.
''PREDICTING RATE OF MASS TRANSFER IN DROP-WISE LIQUID EXTRACTION.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

FOSTER, LEE N.
''A STUDY OF THE RELAXATION OF THE BALESCU-LENARD EQUATIONS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

GARLAND, FRANK
''ULTRASONIC ABSORPTION CALCULATIONS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

GLOCK JR., RUSSELL
''CYLINDRICAL ''VOLUME'' PHASE DELAYED ANTENNA ARRAYS.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

GOEL, NARENDRA
''DENATURATION AND RENATURATION OF DNA MOLECULE.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

HAN, CHANG SUN
''STUDY OF THE B(10) ((HE(3), PA)) BE(8) AND B(10) ((HE(3), A)) B(9*) REACTIONS.''
COLLEGE OF ARTS AND SCIENCES, MASTERS THESIS.

HARRIS, ROBERT N.
''EFFECT OF VIOLATION OF ASSUMPTIONS ON THE T-TEST OF SIGNIFICANCE OF INTERCORRELATIONS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

HARRIS, WILLIAM R.
''ANALYSIS OF C(14)((P,P))C(14) AND N(14)((P,P))N(14).''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

HENDERSON, ANSELM P.
''PILOT STUDY OF GALACTIC BENDING.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

HENDERSON, CHARLES L.
''CONDENSATION OF IMMISCIBLE MIXTURES IN THE PRESENCE OF A NON-CONDENSIBLE GAS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

HIPKINS, DAVID L.
''NEAR FIELD OF ANTENNA.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

HIRST, LESTER L.
''ANOMALOUS FERROMAGNETIC RESONANCE.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

HORD, R. MICHAEL
''EINSTEIN EQUATIONS FOR STATIC, SPHERICALLY SYMMETRIC GEOMETRY WITH COULOMB AND NUCLEAR TYPE FORCES.''
COLLEGE OF ARTS AND SCIENCES, MASTERS THESIS.

KATZIN, JOEL C.
''PCAC CALCULATIONS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

KERN, RICHARD C.
''DETERMINATION OF INTERNAL FLUX DISTRIBUTIONS IN LUMPED HIGHLY ABSORBING MATERIALS USING THE NUCLEAR REACTOR.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

KNIEDLER, MARCEL J.
''ELECTRON ENERGY DEPOSITION.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

KNOPP, LAURENCE I.
''EFFECTIVE REACTIVITY CONTROL BY COMBINATIONS OF NEUTRON ABSORBERS IN NUCLEAR REACTORS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

LATORRE, VICTOR
''ELASTIC SCATTERING OF PROTONS BY C(13) NUCLEUS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

LEE, RICHARD M.
''ACQUISITION OF STABLE PERFORMANCE ON SEVERAL SCHEDULES OF INTERMITTENT REINFORCEMENT.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

LIGHTNER, RALPH G.
''DYNAMIC STUDY OF H-ZR SYSTEM FOR NUCLEAR REACTOR CONTROL.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

LYONS, ROBERT E.
''CALCULATION OF THE RELIABILITY OF REDUNDANT LOGIC NETWORKS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

MAGTOTO, EDUARDO R.
KINETIC STUDY OF ADSORPTION OF 2, 4-D IN WATER BY ACTIVATED CARBON IN A DIFFERENTIAL BED.''
COLLEGE OF ENGINEERING, DOCTORS DISSERTATION.

MARTIN, R. D.
''NETWORK ANALYSIS WITH THE DIGITAL COMPUTER.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

MEHTA, KISHOR K.
''NUCLEAR SPECTROSCOPY USING NUCLEAR REACTOR NEUTRONS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

MO, BENEDICT
''ELASTIC SCATTERING OF PROTONS BY BERYLLIUM 9.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

MOAZED, CYRUS
''MULTI-PARTICLE BREAKUP.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

O'BRIEN, JOHN L.
''SOME EFFECTS OF TEMPERATURE ON THE CRITICALITY OF THE UNIVERSITY OF MARYLAND REACTOR.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

OUYANG, BINYORK
''SHOCK TUBE MEASUREMENT ON RELAXATION TIME OF HYDROGEN.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERATION.

PARK, CHAN M.
''DISPERSION COEFFICIENTS IN FLOW REACTOR VESSELS.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

PEARLSTEIN, ROBERT M.
''THEORY OF CHLOROPHYLL-A FLUORESCENCE IN GREEN PLANT PHOTO-SYNTHESIS.''
COLLEGE OF ARTS AND SCIENCES, MASTERS THESIS.

PERINI, LUIGI L.
''NONEQUILIBRIUM BLUNT BODY FLOW.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

POLLACK, HAROLD
''STUDIES IN TWO-PHASE DOWNFLOW.''
COLLEGE OF ENGINEERING, DOCTOROL DISSERTATION.

REILLY, RICHARD
''PERFORMANCE CHARACTERISTICS OF HYPERSONIC HELIUM TUNNEL.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

RIEGEL, KURT W.
''H II REGION LINE PROFILE ANALYSIS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

ROSS, MALCOLM F.
''RELATIVE REACTIVITY WORTHS OF NEUTRON ABSORBING MATERIALS FOR VARIOUS GEOMETRIES.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

SACHS, AVNER Y.
''UNSTEADY FLOW OVER A FLAT PLATE IN RADIATION GASDYNAMICS.''
COLLEGE OF ARTS AND SCIENCES, MASTERS THESIS.

SAMBAMOORTHY, JAYARAMAN K.
''NUCLEAR REACTION.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

SCHREIER, STEFAN
''NONSTEADY STATE HEAT TRANSFER IN HYPERSONIC FLOW.''
COLLEGE OF ENGINEERING, DOCTORAL DISSERTATION.

SHAFFER, STUART M.
''VARIABILITY OF DETECTION LEVEL IN VISUAL PERCEPTION.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

SMITH, MORTON
''COORDINATE CONVERSION IN THE OMEGA RADIO NAVIGATION SYSTEM.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

STAPLES, BERT R.
''CONDUCTANCE OF CHARGE SEPARATED ELECTROLYTES.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

STOLOFF, PETER
''INVESTIGATION OF THE EFFECTS OF VIOLATING THE ASSUMPTIONS OF THE REPEATED MEASURES DESIGN IN THE ANALYSIS OF VARIANCE.''
COLLEGE OF ARTS AND SCIENCES, MASTERS THESIS.

TAYLOR, LESLIE C.
''EFFECTIVENESS OF ANISOTROPIC RECTANGULAR COOLING FINS.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

THOMPSON, RICHARD C.
''THE KINETICS OF THE OXIDATION OF CHROMIUM (II) BY CHLORATE IN AQUEOUS PERCHLORIC ACID.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

TSAO, CHI-KUNG
''BOUNDARY LAYER FLOW WITH THERMAL RADIATION TRANSFER AT LOW PRANDTL NUMBERS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.

WEISS, ROGER O.
''THE INVESTIGATION OF THE THERMAL STRESSES IN A CONICAL RADOME BY THE METHOD OF FINITE DIFFERENCES.''
COLLEGE OF ENGINEERING, MASTERS THESIS.

YU, VICTOR
''WEAK INTERACTION FORM FACTORS.''
COLLEGE OF ARTS AND SCIENCES, DOCTORAL DISSERTATION.